ANALYSIS OF THE MAGNETIC TRANSLATION GROUP AND INVESTIGATION OF A ONE-DIMENSIONAL TOPOLOGICAL MODEL

A THESIS SUBMITTED TO

THE GRADUATE SCHOOL OF ENGINEERING AND SCIENCE

OF BILKENT UNIVERSITY

IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR

THE DEGREE OF

MASTER OF SCIENCE

IN

PHYSICS

By

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August 2017

Analysis of the magnetic translation group and investigation of a one-dimensional topological model
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August 2017

We certify that we have read this thesis and that in our opinion it is fully adequate, in scope and in quality, as a thesis for the degree of Master of Science.

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ABSTRACT

ANALYSIS OF THE MAGNETIC TRANSLATION GROUP AND INVESTIGATION OF A ONE-DIMENSIONAL TOPOLOGICAL MODEL

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M.S. in Physics
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August 2017

The periodicity of a space lattice in presence of a uniform magnetic field is preserved. During this thesis, we will study a set of modified translation operators which commute with the effective Hamiltonian of an electron in the lattice. Group theory helps us to construct matrix representations of the modified translation operators. These operators form ray groups. Using group projection operators, we will find partner functions for constructed irreducible representation in order to obtain a relation which corresponds to Bloch function in a periodic lattice and is named as Bloch-type function. By multiplying a phase factor to modified translation operators, they will be extended to a new set of operators called magnetic translation operators so that they form a full group rather than a ray group. In a similar procedure, we will investigate displacement operators in phase space coordinate to form a full group of them. In another study, we will introduce a one dimensional model derived from Creutz model, called shifted Creutz model, in which a gap closure appears in its ground state band structure leading to time-reversal symmetry breaking and subsequently giving rise to a topological phase transition. Adopting spin-orbit coupling to our model, generates a time-reversal symmetric pair of states with two-fold degeneracy. A topological investigation will be carried on both models by analyzing the band structures, phase diagram, edge states, symmetries in the models, and calculating the winding number.

Keywords: Magnetic translation group, Bloch functions, phase space translation operators, Creutz model, one dimensional topological model.

ÖZET

MANYETİK ÖTELENME GRUPUNUN ANALİZİ VE BİR BOYUTLU TOPOLOJİK MODELİN İNCELENMESİ

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Düzgün bir manyetik alan varlığında bir uzay örgüsünün periyodikliği korunur. Bu tez çalışmasında, örgüdeki bir elektronun etkin Hamilton işlemcisi ile değişme özelliği olan bir dizi düzeltilmiş ötelenme işlemcilerini çalışacağız. Grup teorisi, düzeltilmiş ötelenme işlemcilerinin matris temsillerini oluşturmamıza yardımcı olur. Bu işlemciler ışın gruplarını oluştururlar. Grup projeksiyon işlemcilerini kullanarak, periyodik bir örgüdeki Bloch fonksiyonuna karşılık gelen ve Bloch tipi fonksiyon olarak adlandırılan bir ilişki elde etmek için inşa edilmiş indirgenemez temsillere eş fonksiyonlar bulacağız. Düzeltilmiş ötelenme işlemcileri bir faz faktörü ile çarpılarak manyetik ötelenme işlemcisi adı verilen yeni bir işlemci kümesine genişletilecek ve böylece bir ışın grubu yerine tam bir grup oluşturulacak. Benzer bir şekilde, faz uzayı koordinatlarındaki yer değiştirme işlemcilerini inceleyerek bunların tam bir grubunu oluşturacağız. Diğer bir çalışmada, zamanda tersine simetri kırılmasına ve ardından bir topolojik faz geçişine sebep olan, taban durumu bant yapısında bir boşluk kapanmasının görüldüğü, kaymış Creutz modeli olarak adlandırılan, Creutz modelinden türemiş tek boyutlu bir model sunacağız. Modelimizde spin-yörünge bağlaşımını benimsemek, iki kat yozlaşmış zamanda tersine dönüşümlü simetrik bir çift durum üretir. Her iki model üzerinde de bant yapıları, faz diyagramı, kenar durumları, simetrileri analiz ederek ve sarım sayısını hesaplayarak topolojik bir inceleme yapılacaktır.

Anahtar sözcükler: Manyetik ötelenme grubu, Bloch fonksiyonu, faz uzayı ötelenme işlemcileri, Creutz modeli, bir boyutlu topolojik model.

Dedicated to my parents and my sister ...

Acknowledgement

I would first like to thank my thesis advisor Assist. Prof. Dr. Balázs Hetényi of the physics department at Bilkent university. Whenever I had some trouble or question about my research, Prof. Hetényi helped me patiently and humbly.

I would also like to thank Mohammad Yahyavi, PhD student of Prof. Hetényi who helped me frequently during my research as a friend and colleague.

Finally, I must express my very profound gratitude to my parents for supporting me throughout my years of study and specially these last three years that I stayed away from home.

Sina Gholizadeh.

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Chapter 1

Introduction

1.1 Generalized Bloch functions in uniform magnetic field

The behavior of electrons in crystals is in principle a many-body problem, but we can reduce it to an effective one-body one in which an electron moves in a periodic potential. Bloch functions are consequence of Hamiltonian invariance under lattice translation operators and they are very well-known in solid state physics and condensed matter theory. Lattice translation operators form a full group and it is an easy job to find a matrix representation in finite dimensions. However, when a uniform magnetic field is applied to the lattice, although the Hamiltonian is no longer invariant under the translation group, the periodicity of potential is still not destroyed. In a paper, E. Brown [1] shows that translation operators can be modified by adding a term proportional to the vector potential, in order to commute with Hamiltonian. Unlike usual translation operators, modified translation operators form ray groups rather than full group. Using powerful tools of group theory, Brown shows that by applying Born-von-Karman boundary condition one can construct a matrix representation for the lattice in the presence of uniform magnetic field. By taking the advantages of theorems in group theory,

Brown obtains an equation which corresponds to Bloch functions in the presence of a uniform magnetic field. Few months later, in another paper, J. Zak [2] defines a new set of operators where it has combined modified translation operators with an additional phase factor helping to form a full group. The newly defined operators are called magnetic translation operators and the group that they are generating is called magnetic translation group. In our work, we investigate a set of translation operators in phase space coordinate called displacement operators. These operators form a ray group, however we can modify these operators by adding a new phase factor to generate a full group of them.

1.2 Shifted Creutz model with spin-orbit coupling

After discovery of Hall effect at 1879 by Edwin H. Hall, the measurements on Hall resistance in ferromagnetic and paramagnetic metal in a magnetic field showed that there is an additional contribution to Hall resistance. It took a long time to describe this anomalous physical behavior where it is originating from a relativistic quantum mechanical effect in which the spin and orbital angular momentum of electrons are coupled. This effect leads electrons to feel a spin-dependent force while they are traveling in the crystal. We can still observe this effect, called spin Hall effect, in absence of an external magnetic field and even in non-magnetic materials. In 1980, in an experimental discovery, it is shown that in a two dimensional electron gas subjected to a strong magnetic field there exist a plateau of Hall conductivity proportional to an integer prefactor value while the conductance along the material is zero. This effect is called integer quantum Hall effect and it is shown later by Haldane [3] that this effect can also be a result of electrons band structure while the pure magnetic flux is zero. The quantum spin Hall effect was developed by Kane and Mele [4, 5] who applied spin-orbit interaction to the model suggested earlier by Haldane. In their model, they depicted the quantum spin Hall effect as a combination of two opposite-chirality spin-up and spin-down with vanishing charge Hall conductance but a quantized spin-Hall

conductance. As a consequence, electrons with spin up and spin down move in opposite directions around the edges of the material while it behaves as insulator in the bulk. The quantum spin Hall effect preserves the time reversal symmetry and it is also dubbed as 2D topological insulator.

In Creutz model, the isolated states can be seen when a cross-linked ladder model is under a magnetic field. In presence of a magnetic field, some phases emerge when electrons is hopping from one chain to another. In this model, phases are considered on horizontal bonds in which only first nearest neighborhood is taken into account. In this system, the placed electron will hop from a site to another while it is losing energy because of dissipation, finally, it will settle into ground state with a wavefunction which is not zero in every site. The Hamiltonian given in Creutz [6] model, is showing some symmetries. These symmetries are helpful in studying the energy structure of the system. Our model is shifted Creutz-model with appearing phases on diagonal bonds. The Hamiltonian for new model will be studied both numerically and analytically. Recently, a huge effort is started to classify electronic states based on topological behaviors. There are methods developed and discussed in order to study the spin-orbit interaction in solid state systems. Kane and Mele [4, 5] studied the effects of spin-orbit interaction in 2D layer of graphene in low energies and they demonstrated how including the spin-orbit interactions leads a semimetallic state converts to quantum spin Hall insulator. Similarly, we rewrite our Hamiltonian, while spin-orbit interaction is considered, to study its effects on our model whether it adds new symmetries or breaks the symmetries.

Chapter 2

Lattice in a magnetic field

2.1 Bloch functions

Electron behavior in a periodic potential of a crystal is a many-body problem in general. Here, we assume that electrons have no interaction with nuclei and other electrons. By taking the advantage of periodicity of the potential in an ideal crystal, we can reduce our problem to a single electron problem whose the Hamiltonian is invariant under lattice translation. We consider the periodic potential as,

$$V(\mathbf{r}+\mathbf{R}) = V(\mathbf{r}) \tag{2.1}$$

for all Bravais lattice vectors $\mathbf{R}$. And effective Hamiltonian would be defined as following,

$$H\psi = \left[\frac{p^2}{2m} + V(\mathbf{r})\right]\psi = E\psi. \tag{2.2}$$

Electrons obeying the mentioned Hamiltonian are known as Bloch Electrons. Now, let's define a translation operator denoted by T_R where each of them is corresponding to a Bravais lattice vector $\mathbf{R}$ as following,

$$T_R f(\mathbf{r}) = f(\mathbf{r}+\mathbf{R}). \tag{2.3}$$

It can be confirmed that periodic Hamiltonian and defined translation operator commute,

$$[H, T_R] = 0, \tag{2.4}$$

as well as two successive translation operators for different vectors of $\mathbf{R}$ and $\mathbf{R}'$,

$$[T_R, T_{R'}] = 0 \quad \text{and} \quad T_R T_{R'} = T_{R'} T_R = T_{R+R'}. \tag{2.5}$$

It follows from quantum mechanics that the eigenfunctions of H can be chosen in a way to be simultaneous eigenfunctions of all the T_R:

$$\begin{aligned} H\psi &= E\psi \\ T_R\psi &= c(\mathbf{R})\psi. \end{aligned} \tag{2.6}$$

Since the translation operators commute, following 2.5, we have:

$$c(\mathbf{R} + \mathbf{R}') = c(\mathbf{R})c(\mathbf{R}'). \tag{2.7}$$

Let's define the Bravais lattice's primitive vectors as $\mathbf{a}_i$ where $i = 1, 2, 3$. Then we can always write the $c(\mathbf{a}_i)$ in the form

$$c(\mathbf{a}_i) = e^{2\pi i x_i}, \tag{2.8}$$

if we take $\mathbf{R}$ in its general form of,

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \tag{2.9}$$

then by successive application of 2.7 we have,

$$c(\mathbf{R}) = c(\mathbf{a}_1)^{n_1} c(\mathbf{a}_2)^{n_2} c(\mathbf{a}_3)^{n_3} \tag{2.10}$$

and this is equivalent to

$$c(\mathbf{R}) = e^{i\mathbf{k}.\mathbf{R}}, \tag{2.11}$$

where

$$\mathbf{k} = x_1\mathbf{b}_1 + x_2\mathbf{b}_2 + x_3\mathbf{b}_3 \tag{2.12}$$

and $\mathbf{b}_i$ are three reciprocal primitive vectors. We have following condition,

$$\mathbf{b}_i.\mathbf{a}_j = 2\pi\delta_{ij}. \tag{2.13}$$

So far we have shown that the eigenfunctions satisfying equation 2.6 can be expressed as following,

$$T_R\psi(\mathbf{r}) = \psi(\mathbf{r}+\mathbf{R}) = c(\mathbf{R})\psi(\mathbf{r}) = e^{i\mathbf{k}.\mathbf{R}}\psi(\mathbf{r}) \tag{2.14}$$

which is exactly one of the forms of Bloch's theorem. We have not specified that whether $\mathbf{k}$ is a complex or real vector. Since the probability of finding an electron is same at points $\mathbf{r}$ and $\mathbf{r}+\mathbf{R}$ in an infinite size lattice, hence we expect that,

$$\begin{aligned} &\int \psi^*(\mathbf{r})\psi(\mathbf{r})d^3r = 1 \\ &= \int \psi^*(\mathbf{r}+\mathbf{R})\psi(\mathbf{r}+\mathbf{R})d^3r = c^*(\mathbf{R})c(\mathbf{R})\int \psi^*(\mathbf{r})\psi(\mathbf{r})d^3r = 1 \end{aligned} \tag{2.15}$$

in which $c^*(\mathbf{R})c(\mathbf{R}) = 1$ guarantees that $\mathbf{k}$ is a real vector. We can write Bloch's theorem in one dimensional form by rewriting equation 2.12 in the following way,

$$\mathbf{k} = \mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3, \tag{2.16}$$

then for a single step displacement in $\mathbf{a}_1$ direction, Bloch's theorem will be,

$$T_{a_1}\psi = \psi(x_1 + a_1) = e^{ik_1a_1}\psi(x_1). \tag{2.17}$$

Another approach to obtain Bloch's theorem in a finite size lattice is given by group theory. Consider a one-dimensional Hamiltonian with a periodic potential arranged in a linear way and associated with periodic boundary conditions applied at edges with h separated periodic parts. It can be shown that the cyclic group of order h is the symmetry group of the described Hamiltonian. We define the generator of the cyclic group to be A representing a translation for one period of size a. We assign a linear operator T_A corresponding to translation A where it acts on function $\psi(x)$,

$$T_A\psi(x) = \psi(x+a). \tag{2.18}$$

If we apply translation linear operator[1] for h times to the eigenfunctions of the Hamiltonian,

$$T_A^h\psi(x) = \psi(x+ha) = \psi(x) \tag{2.19}$$

so, T_A can be written as h'th root of unity,

$$T_A = e^{2\pi ip/h}, \qquad p = 1, 2, 3, \ldots, h, \tag{2.20}$$

[1]Since now we will continue calling translation operator instead of full name.

or in another words,

$$T_A\psi(x) = \psi(x+a) = e^{2\pi ip/h}\psi(x). \tag{2.21}$$

Let's assume that the total length of linear arrangement is $L = ah$. Then we can write,

$$T_A\psi(x) = \psi(x+a) = e^{2\pi ipa/L}\psi(x) = e^{ika}\psi(x) \tag{2.22}$$

where k is related to p by $k = 2\pi p/L$.

Up to this point, we figured out how to obtain Bloch functions for a lattice with a periodic potential in different ways. Now a question can be asked and that is "do there exist functions similar to Bloch functions expressing the electrons behavior in a lattice in presence of a uniform magnetic field?"

To answer this question we should rewrite the introduced effective Hamiltonian consistent with magnetic field,

$$H = \frac{1}{2m}\left(\mathbf{p} + \frac{e\mathbf{A}}{c}\right)^2 + V(\mathbf{r}) \tag{2.23}$$

where $\mathbf{A}$ is vector potential and is given in the following gauge,

$$\mathbf{A} = -\frac{1}{2}(\mathbf{r} \times \mathbf{B}). \tag{2.24}$$

Different components of $(\mathbf{p} + e\mathbf{A}/c)$ are not commuting,

$$[(\mathbf{p} + e\mathbf{A}/c)_i, (\mathbf{p} + e\mathbf{A}/c)_j] \neq 0 \quad ; \quad i,j = 1,2,3 \tag{2.25}$$

while the components of $(\mathbf{p} - e\mathbf{A}/c)$ is commuting with $(\mathbf{p} + e\mathbf{A}/c)$,

$$[(\mathbf{p} - e\mathbf{A}/c)_i, (\mathbf{p} + e\mathbf{A}/c)_j] = 0 \quad ; \quad i,j = 1,2,3. \tag{2.26}$$

Equation 2.26 helps us to define a new translation operator according to $(\mathbf{p} - e\mathbf{A}/c)$,

$$T(\mathbf{R_n}) = \exp[-i\mathbf{R_n} \cdot (\mathbf{p} - e\mathbf{A}/c)/\hbar] \tag{2.27}$$

where its effect on an arbitrary function is,

$$T(\mathbf{R_n})\psi(\mathbf{r}) = \exp[+i(\mathbf{R_n} \times \boldsymbol{\beta}) \cdot \mathbf{r}/2]\psi(\mathbf{r} - \mathbf{R_n}) \tag{2.28}$$

in which $\boldsymbol{\beta} = e\mathbf{B}/\hbar c$, while the translation operator without magnetic field would be:

$$\begin{aligned} \mathrm{T}(\mathbf{R_n}) &= \exp[-i\mathbf{R_n}\cdot\mathbf{p}/\hbar] \\ \mathrm{T}(\mathbf{R_n})\psi(\mathbf{r}) &= \psi(\mathbf{r}-\mathbf{R_n}). \end{aligned} \tag{2.29}$$

Modified translation operators don't commute with each other,

$$\begin{aligned} T(\mathbf{R_1})T(\mathbf{R_2}) &= T(\mathbf{R_2})T(\mathbf{R_1})\exp[-i(\mathbf{R_1}\times\mathbf{R_2})\cdot\boldsymbol{\beta}] \\ T(\mathbf{R_1})T(\mathbf{R_2}) &= T(\mathbf{R_1}+\mathbf{R_2})\exp[(-i/2)(\mathbf{R_1}\times\mathbf{R_2})\cdot\boldsymbol{\beta}]. \end{aligned} \tag{2.30}$$

Modified translation operators generate ray group rather than a group and this is because of the phase factor that appears in the second part of 2.30. These operators are basic to magnetic field problems. It can be shown that Hamiltonian and modified translation operator are commuting,

$$[H, T(\mathbf{R_n})] = 0. \tag{2.31}$$

Since Hamiltonian and translation operator commute, we can choose a simultaneous eigenbasis for them. Let's have an energy eigenvalue which is M-fold degenerate associated with eigenfunctions ψ_m,

$$T(\mathbf{R_n})\psi_m = \sum_{l=1}^{M} D_{lm}(\mathbf{R_n})\psi_l \tag{2.32}$$

After working a while on equations 2.30 and 2.32, it can be figured out that:

$$D(\mathbf{R_1})D(\mathbf{R_2}) = D(\mathbf{R_1}+\mathbf{R_2})\exp[(-i/2)(\mathbf{R_1}\times\mathbf{R_2})\cdot\boldsymbol{\beta}] \tag{2.33}$$

In order to demonstrate translation operators with matrix representations , we need to reduce our system to a finite size and consequently the ray group will reduce to a finite size group as well. Let's assume $\mathbf{a_1}, \mathbf{a_2}, \mathbf{a_3}$ are primitive translation operators. The dimensions of the finite lattice is defined by $N_1\mathbf{a_1}, N_2\mathbf{a_2}, N_3\mathbf{a_3}$. Applying Born-Von Karman boundary condition to a finite lattice in absence of the magnetic field(zero-field), is to impose a restriction on the eigenfunctions to be periodic for a certain Bravais lattice vectors,

$$T(N_i\mathbf{a_i})\psi = \psi \quad ; \quad i = 1, 2, 3. \tag{2.34}$$

We can invoke the same boundary condition in the presence of a uniform magnetic field. But there is a difference with zero-field case. Here the eigenfunction obtained from a translation operator $T(\mathbf{R_m})$, applied on ψ, is not going into itself by undergoing the translation operator of $T(N_i\mathbf{a_i})$,

$$\phi_m = T(\mathbf{R_m})\psi. \tag{2.35}$$

Using equation 2.30 we have,

$$T(N_i\mathbf{a_i})\phi_m = \exp[-iN_i(\mathbf{a_i} \times \mathbf{R_m}) \cdot \boldsymbol{\beta}]\phi_m. \tag{2.36}$$

In order to having the boundary condition applied to all the functions, we require that,

$$N_i(\mathbf{a_i} \times \mathbf{R_m}) \cdot \boldsymbol{\beta} = \text{ multiple of } 2\pi \tag{2.37}$$

Question: What form $\boldsymbol{\beta}$ should have to satisfy the condition given by equation 2.37?
Since $\mathbf{R}_m$ is a Bravais lattice vector, hence we can express it in the form of,

$$\mathbf{R}_m = \sum_i n_i^{(m)} \mathbf{a}_i \tag{2.38}$$

Now, in order to be consistent with magnetically periodic boundary condition, we are assuming $\boldsymbol{\beta}$ in the following form:

$$\boldsymbol{\beta} = \alpha \mathbf{R} \tag{2.39}$$

where $\mathbf{R} = \sum_i n_i \mathbf{a}_i$ is a primitive lattice vector. After canceling out the common factors, $\boldsymbol{\beta}$ is given by:

$$\boldsymbol{\beta} = 2\pi l \frac{1}{N\Omega} \mathbf{R} \tag{2.40}$$

where l, N are integer numbers which provide a rational number l/N and Ω is the volume of a primitive cell.

The magnetic translation operators are unitary. If we choose an orthonormal basis, then we can construct a unitary matrix representation for operators. We choose $\boldsymbol{\beta}$ to be alongside vector $\mathbf{a}_3$ without loss in generality,

$$\boldsymbol{\beta} = 2\pi l \frac{1}{N\Omega} \mathbf{a}_3. \tag{2.41}$$

Using 2.30 commutation relations for primitive vectors would lead to,

$$\begin{aligned}
&[T(\mathbf{a}_3), T(\mathbf{a}_1)] = [T(\mathbf{a}_3), T(\mathbf{a}_2)] = 0 \\
&T(\mathbf{a}_1)T(\mathbf{a}_2) = \exp\Big(-i\frac{2\pi l}{N}\Big)T(\mathbf{a}_2)T(\mathbf{a}_1),
\end{aligned} \tag{2.42}$$

it can be figured out from 2.42 that we are restricted from below to a size given by two dimensional N by N structure with one unit cell thickness in the $\mathbf{a}_3$ direction, while magnetically periodic boundary conditions is imposed. This domain is called as magnetic unit cell. Two dimensional N by N plane is spanned by $\mathbf{a}_1$ and $\mathbf{a}_2$, thus the group consists of N^2 operations.

According to equation 2.42 $T(\mathbf{a}_3)$ is commuting with both $T(\mathbf{a}_1)$ and $T(\mathbf{a}_2)$, therefore it makes sense to take it as an identity matrix with order of N by N. Let's invoke equation 2.32,

$$T(\mathbf{R_n})\psi_m = \sum_{l=1}^{M} D_{lm}(\mathbf{R_n})\psi_l$$

by replacing $\mathbf{a}_3$ instead of $\mathbf{R_n}$ and few changes, we are left with,

$$T(\mathbf{a}_3)\psi_k = \sum_{j=1}^{N} D_{jk}(\mathbf{a}_3)\psi_j = \sum_{j=1}^{N} \delta_{jk}\psi_j = \psi_k \tag{2.43}$$

In next steps, we will try to find the matrix representations for $T(\mathbf{a}_1)$ and $T(\mathbf{a}_2)$. We use the same equation 2.32,

$$\begin{aligned}
T(\mathbf{a}_1)\psi_k &= \sum_{j=1}^{N} D_{jk}(\mathbf{a}_1)\psi_j \\
T(\mathbf{a}_2)\psi_k &= \sum_{j=1}^{N} D_{jk}(\mathbf{a}_2)\psi_j \\
T(\mathbf{a}_1)T(\mathbf{a}_2)\psi_k &= \exp\Big(-i\frac{2\pi l}{N}\Big)T(\mathbf{a}_2)T(\mathbf{a}_1)\psi_k
\end{aligned} \tag{2.44}$$

applying $T(\mathbf{a}_2)$ in the left side and $T(\mathbf{a}_1)$ in the right side of the equation to ψ_k gives us,

$$\begin{aligned}
&T(\mathbf{a}_1)[D_{1k}(\mathbf{a}_2)\psi_1 + D_{2k}(\mathbf{a}_2)\psi_2 + \ldots + D_{Nk}(\mathbf{a}_2)\psi_N] = \\
&\exp\Big(-i\frac{2\pi l}{N}\Big)T(\mathbf{a}_2)[D_{1k}(\mathbf{a}_1)\psi_1 + D_{2k}(\mathbf{a}_1)\psi_2 + \ldots + D_{Nk}(\mathbf{a}_1)\psi_N]
\end{aligned} \tag{2.45}$$

and applying $T(\mathbf{a}_1)$ in the left side and $T(\mathbf{a}_2)$ in the right side of the equation to the terms inside the brackets,

$$\begin{aligned}
&\Rightarrow D_{1k}(\mathbf{a}_2)T(\mathbf{a}_1)\psi_1 + D_{2k}(\mathbf{a}_2)T(\mathbf{a}_1)\psi_2 + \ldots + D_{Nk}(\mathbf{a}_2)T(\mathbf{a}_1)\psi_N = \\
&\quad \exp\Big(-i\frac{2\pi l}{N}\Big)\Big[D_{1k}(\mathbf{a}_1)T(\mathbf{a}_2)\psi_1 + D_{2k}(\mathbf{a}_2)T(\mathbf{a}_2)\psi_2 + \ldots + D_{Nk}(\mathbf{a}_1)T(\mathbf{a}_2)\psi_N\Big]
\end{aligned} \tag{2.46}$$

and after expanding it,

$$\begin{aligned}
&\Rightarrow D_{1k}(\mathbf{a}_2)[D_{11}(\mathbf{a}_1)\psi_1 + D_{21}(\mathbf{a}_1)\psi_2 + \ldots + D_{N1}(\mathbf{a}_1)T(\mathbf{a}_1)\psi_N \\
&\quad + \ldots + D_{Nk}(\mathbf{a}_2)[D_{1N}(\mathbf{a}_1)\psi_1 + D_{2N}(\mathbf{a}_1)\psi_2 + \ldots + D_{NN}(\mathbf{a}_1)\psi_N] \\
&\quad = \exp\Big(-i\frac{2\pi l}{N}\Big)\Big\{D_{1k}(\mathbf{a}_1)[D_{11}(\mathbf{a}_2)\psi_1 + D_{21}(\mathbf{a}_2)\psi_2 + \ldots + D_{N1}(\mathbf{a}_1)\psi_N] \\
&\quad + \ldots + D_{Nk}(\mathbf{a}_1)[D_{1N}(\mathbf{a}_2)\psi_1 + D_{2N}(\mathbf{a}_2)\psi_2 + \ldots + D_{NN}(\mathbf{a}_2)\psi_N]\Big\}
\end{aligned} \tag{2.47}$$

Now, it is time to rearrange the terms according to ψ_1, ψ_2 and etc:

$$\begin{aligned}
&[D_{1k}(\mathbf{a}_2)D_{11}(\mathbf{a}_1) + D_{2k}(\mathbf{a}_2)D_{12}(\mathbf{a}_1) + \ldots + D_{Nk}(\mathbf{a}_2)D_{1N}(\mathbf{a}_1)]\psi_1 \\
&+ [D_{1k}(\mathbf{a}_2)D_{21}(\mathbf{a}_1) + D_{2k}(\mathbf{a}_2)D_{22}(\mathbf{a}_1) + \ldots + D_{Nk}(\mathbf{a}_2)D_{2N}(\mathbf{a}_1)]\psi_2 \\
&+ \ldots \\
&+ [D_{1k}(\mathbf{a}_2)D_{N1}(\mathbf{a}_1) + D_{2k}(\mathbf{a}_2)D_{N2}(\mathbf{a}_1) + \ldots + D_{Nk}(\mathbf{a}_2)D_{NN}(\mathbf{a}_1)]\psi_N \\
&= \exp\Big(-i\frac{2\pi l}{N}\Big)\Big\{[D_{1k}(\mathbf{a}_1)D_{11}(\mathbf{a}_2) + D_{2k}(\mathbf{a}_1)D_{12}(\mathbf{a}_2) + \ldots + D_{Nk}(\mathbf{a}_1)D_{1N}(\mathbf{a}_2)]\psi_1 \\
&+ [D_{1k}(\mathbf{a}_1)D_{21}(\mathbf{a}_2) + D_{2k}(\mathbf{a}_1)D_{22}(\mathbf{a}_2) + \ldots + D_{Nk}(\mathbf{a}_1)D_{2N}(\mathbf{a}_2)]\psi_2 \\
&+ \ldots \\
&+ [D_{1k}(\mathbf{a}_1)D_{N1}(\mathbf{a}_2) + D_{2k}(\mathbf{a}_1)D_{N2}(\mathbf{a}_2) + \ldots + D_{Nk}(\mathbf{a}_1)D_{NN}(\mathbf{a}_2)]\psi_N\Big\},
\end{aligned} \tag{2.48}$$

we will assume that $D_{jk}(\mathbf{a}_1)$ is a diagonal matrix while the non-zero arrays of the matrix $D_{jk}(\mathbf{a}_2)$ is arranged according to $\delta_{j,k-1}(\text{mod } N)$.

$$\begin{aligned}
D_{jk}(\mathbf{a}_1) &= \delta_{jk} f(j) \\
D_{jk}(\mathbf{a}_2) &= \delta_{j,k-1} \pmod N.
\end{aligned} \tag{2.49}$$

Since $\{\psi_i\}_{i=1}^{N}$ is a set of linearly independent vectors, hence we can compare coefficient of each ψ_i separately on both sides:

If we consider $k = 1$ in 2.48, then we are left with no terms at both sides, while for $k = 2$, we are left with coefficients of ψ_1 at both sides:

$$D_{12}(\mathbf{a}_2)D_{11}(\mathbf{a}_1) = \exp\Big(-i\frac{2\pi l}{N}\Big)D_{22}(\mathbf{a}_1)D_{12}(\mathbf{a}_2) \tag{2.50}$$

and for $k = 3$, we are left with coefficients of ψ_2 at both sides:

$$D_{23}(\mathbf{a}_2)D_{22}(\mathbf{a}_1) = \exp\Big(-i\frac{2\pi l}{N}\Big)D_{33}(\mathbf{a}_1)D_{23}(\mathbf{a}_2) \tag{2.51}$$

then by setting $D_{11}(\mathbf{a}_1) = 1$, we can claim:

$$\begin{aligned} D_{jk}(\mathbf{a}_1) &= \delta_{jk}\exp\Big(i(j-1)\frac{2\pi l}{N}\Big) \quad (j,k = 1,2,...,N) \\ D_{jk}(\mathbf{a}_2) &= \delta_{j,k-1} \qquad (\text{mod N}). \end{aligned} \tag{2.52}$$

Up to this point, we found the matrix representation for primitive vectors. In order to generalize the matrix representation to an arbitrary Bravais lattice vector in two dimensional plane constructed by $\mathbf{a}_1$ and $\mathbf{a}_2$, we invoke equation 2.33,

$$D(\mathbf{R_1})D(\mathbf{R_2}) = D(\mathbf{R_1}+\mathbf{R_2})\exp[(-i/2)(\mathbf{R_1}\times\mathbf{R_2})\cdot\boldsymbol{\beta}].$$

For primitive vector $\mathbf{a}_1$,

$$\begin{aligned} D(\mathbf{a}_1)D(\mathbf{a}_1) &= D(\mathbf{a}_1+\mathbf{a}_1)\exp[(-i/2)(\mathbf{a}_1\times\mathbf{a}_1)\cdot\boldsymbol{\beta}] \\ &= D(\mathbf{a}_1+\mathbf{a}_1) = D(2\mathbf{a}_1), \end{aligned} \tag{2.53}$$

in terms of matrices,

$$\begin{aligned} &\sum_m D_{j,m}(\mathbf{a}_1)D_{m,k}(\mathbf{a}_1) = D_{j,k}(2\mathbf{a}_1) \\ &\Rightarrow \sum_m \delta_{j,m}\exp\Big(i(j-1)\frac{2\pi l}{N}\Big)\delta_{m,k}\exp\Big(i(m-1)\frac{2\pi l}{N}\Big) \\ &= D_{j,k}(2\mathbf{a}_1) \\ &\Rightarrow \delta_{j,k}\Big[\exp\Big(i(j-1)\frac{2\pi l}{N}\Big)\Big]^2 = D_{j,k}(2\mathbf{a}_1), \\ &\text{or} \\ &\Rightarrow [D_{j,k}(\mathbf{a}_1)]^2 = D_{j,k}(2\mathbf{a}_1), \end{aligned} \tag{2.54}$$

after few more steps, it can be shown that,

$$
\begin{aligned}
&[D_{j,k}(\mathbf{a}_1)]^{n_1} = D_{j,k}(n_1\mathbf{a}_1),\\
&\text{or}\\
&D_{j,k}(n_1\mathbf{a}_1) = \delta_{j,k}\exp\Big(i(j-1)\frac{2\pi l n_1}{N}\Big).
\end{aligned}
\tag{2.55}
$$

To find the matrix representation for $n_2\mathbf{a}_2$,

$$
\begin{aligned}
&\sum_m D_{j,m}(\mathbf{a}_2)D_{m,k}(\mathbf{a}_2) = D_{j,k}(\mathbf{a}_2+\mathbf{a}_2)\\
&\Rightarrow \sum_m \delta_{j,m-1}\delta_{m,k-1} = D_{j,k}(2\mathbf{a}_2)\\
&\Rightarrow \delta_{j,k-2} = D_{j,k}(2\mathbf{a}_2),
\end{aligned}
\tag{2.56}
$$

if we continue last step once more,

$$
\begin{aligned}
&D(\mathbf{a}_2)D(2\mathbf{a}_2) = D(3\mathbf{a}_2)\\
&\Rightarrow \sum_m D_{j,m}(\mathbf{a}_2)D_{m,k}(2\mathbf{a}_2) = D_{j,k}(3\mathbf{a}_2)\\
&\Rightarrow \sum_m \delta_{j,m-1}\delta_{m,k-2} = D_{j,k}(3\mathbf{a}_2)\\
&\Rightarrow \delta_{j,k-3} = D_{j,k}(3\mathbf{a}_2),
\end{aligned}
\tag{2.57}
$$

based on principle of induction, we can claim,

$$
D_{j,k}(n_2\mathbf{a}_2) = \delta_{j,k-n_2}. \tag{2.58}
$$

What can be the matrix representation for a Bravais lattice in the plane of vectors $\mathbf{a}_1$ and $\mathbf{a}_2$? We recall equation 2.33 another time, and replace $\mathbf{R}_1$ with $n_1\mathbf{a}_1$ and

$\mathbf{R}_2$ with $n_2\mathbf{a}_2$. Let's write the equation in indices form,

$$\sum_m D_{j,m}(n_1\mathbf{a}_1)D_{m,k}(n_2\mathbf{a}_2) = D_{j,k}(n_1\mathbf{a}_1 + n_2\mathbf{a}_2)\exp\Big[(-i/2)(n_1\mathbf{a}_1 \times n_2\mathbf{a}_2)\cdot\boldsymbol{\beta}\Big]$$

$$\Rightarrow \sum_m \delta_{j,m}\exp\Big(i(j-1)\frac{2\pi l n_1}{N}\Big)\delta_{m,k-n_2} = D_{j,k}(n_1\mathbf{a}_1 + n_2\mathbf{a}_2)\exp\Big[(-i/2)(n_1\mathbf{a}_1 \times n_2\mathbf{a}_2)\cdot\boldsymbol{\beta}\Big]$$

$$\Rightarrow \sum_m \delta_{j,m}\exp\Big(i(j-1)\frac{2\pi l n_1}{N}\Big)\delta_{m,k-n_2}$$

$$= D_{j,k}(n_1\mathbf{a}_1 + n_2\mathbf{a}_2)\exp\Big[(-i/2)(n_1\mathbf{a}_1 \times n_2\mathbf{a}_2)\cdot\Big(\frac{2\pi l}{\Omega N}\Big)\mathbf{a}_3\Big]$$

$$= D_{j,k}(n_1\mathbf{a}_1 + n_2\mathbf{a}_2)\exp\Big[(-i)(n_1 n_2)\Big(\frac{\pi l}{N}\Big)\Big]$$

$$\Rightarrow \delta_{j,k-n_2}\exp\Big(i(j-1)\frac{2\pi l n_1}{N}\Big) = D_{j,k}(n_1\mathbf{a}_1 + n_2\mathbf{a}_2)\exp\Big[(-i)(n_1 n_2)\Big(\frac{\pi l}{N}\Big)\Big]$$

$$\Rightarrow \delta_{j,k-n_2}\exp\Big[\frac{i\pi l n_1}{N}\big(n_2 + 2(j-1)\big)\Big] = D_{j,k}(n_1\mathbf{a}_1 + n_2\mathbf{a}_2)$$

or

$$D_{j,k}(n_1\mathbf{a}_1 + n_2\mathbf{a}_2) = \delta_{j,k-n_2}\exp\Big[\frac{i\pi l n_1}{N}\big(n_2 + 2(j-1)\big)\Big]. \tag{2.59}$$

The orthogonality relation. If all nonequivalent irreducible representations(irrep) of a group G is considered, μ and ν denote nonequivalent irreps, then the quantities $D^{(\mu)}_{i,j}(R)(i,j = 1,2,\ldots,n_\mu)$, for fixed values of μ, i, j form a vector in a g-dimensional[2] space:

$$\sum_R D^{(\mu)}_{i,l}(R)D^{(\nu)}_{m,j}(R^{-1}) = \frac{g}{n_\mu}\delta_{\mu\nu}\delta_{ij}\delta_{lm}, \tag{2.60}$$

if the considered representation is unitary, we also can write,

$$\sum_R D^{(\mu)}_{i,l}(R)D^{(\nu)*}_{m,j}(R) = \frac{g}{n_\mu}\delta_{\mu\nu}\delta_{ij}\delta_{lm}. \tag{2.61}$$

Each irreducible representation $D^{(\mu)}$ gives us n_μ^2 orthogonal vectors which are also orthogonal to the provided vectors of all the other nonequivalent irreps,

$$\sum_\mu n_\mu^2 = g. \tag{2.62}$$

[2]g: order of group G

In addition, a similar equation can be derived for characters of $D^{\mu}(R)$,

$$\sum_{R} \chi^{(\mu)}(R)\chi^{(\nu)*}(R) = g\delta_{\mu\nu}. \tag{2.63}$$

Let's recall equation 2.59,

$$D_{j,k}(n_1\mathbf{a}_1 + n_2\mathbf{a}_2) = \delta_{j,k-n_2} \exp\Big[\frac{i\pi l n_1}{N}\big(n_2 + 2(j-1)\big)\Big], \tag{2.64}$$

it easily can be seen that the traces D_{ii} of all the matrices are zero, except the identity which has a trace of N,

$$\sum_{i=1}^{N} D_{ii}(\mathbf{a}_3) = \sum_{i=1}^{N} \delta_{ii} = N. \tag{2.65}$$

So, the sum of the squares of the traces is N^2, which is order of the group. Therefore, the representation is irreducible. Moreover, the square of its dimension is also N^2,

$$\sum_{\mu} n_{\mu}^2 = N^2 = g, \tag{2.66}$$

which means there can be no other nonequivalent irreducible representation.
The group that we constructed under magnetically periodic boundary condition has N^2 elements. In the magnetic unit cell that we considered, only irreducible representation of dimensionality N can be found where its eigenvalues are N-fold degenerate.

Let's consider a function ψ in which we can construct a representation by applying all the transformations of the group G to the ψ. Either ψ is itself one of the base functions of the constructed representation or it is a linear combination of the base functions. If we split the representation into its irreducible representations, our claim is still valid,

$$\psi = \sum_{\nu} \sum_{i=1}^{n_\nu} \psi_i^{(\nu)}, \tag{2.67}$$

where $\{\psi_i^{(\nu)}\}_{i=1}^{n_\nu}$ provides the base functions for νth irreducible representation. The linear operators O_R correspond to elements R of the group G, and they

satisfy,

$$O_R\psi_i^{(\nu)} = \sum_j \psi_j^{(\nu)} D_{ji}^{(\nu)}(R). \tag{2.68}$$

Now, finding the condition for the base functions of a given representation in order to satisfy the equation 2.68 is a matter of question. Let's multiply 2.68 by $D_{lm}^{(\mu)*}(R)$ and sum over the elements of the group:

$$\begin{aligned} \sum_R D_{lm}^{(\mu)*}(R) O_R \psi_i^{(\nu)} &= \sum_j \psi_j^{(\nu)} \sum_R D_{lm}^{(\mu)*}(R) D_{ji}^{(\nu)}(R) \\ &= \frac{g}{n_\nu} \sum_j \psi_j^{(\nu)} \delta_{lj}\delta_{mi}\delta_{\mu\nu} = \frac{g}{n_\nu}\psi_l^{(\nu)}\delta_{mi}\delta_{\mu\nu}, \end{aligned} \tag{2.69}$$

setting $m = l$, and $\mu = \nu$,

$$\sum_R D_{ll}^{(\nu)*}(R) O_R \psi_i^{(\nu)} = \frac{g}{n_\nu}\psi_l^{(\nu)}\delta_{li}, \tag{2.70}$$

and for specific $l = i$ it gives,

$$\sum_R D_{ii}^{(\nu)*}(R) O_R \psi_i^{(\nu)} = \frac{g}{n_\nu}\psi_i^{(\nu)}, \tag{2.71}$$

Equation 2.71 is a necessary condition for $\psi_i^{(\nu)}$ to be a base function for νth irreducible representation. If the function $\psi_i^{(\nu)}$ satisfies the condition, then we can find $(n_\nu - 1)$ partner functions so that the set provides a base functions for 2.68.

What if instead of a particular function like $\psi_i^{(\nu)}$, we are given a general function like ψ? We can show that the function ψ can be written as sum of the base functions of some of the irreducible representations. Let's set $m = l$ at 2.69,

$$\sum_R D_{ll}^{(\mu)*}(R) O_R \psi_i^{(\nu)} = \frac{g}{n_\mu}\psi_l^{(\nu)}\delta_{li}\delta_{\mu\nu}. \tag{2.72}$$

It is easy to see that the operator,

$$P_i^{(\mu)} = \frac{n_\mu}{g}\sum_R D_{ii}^{(\mu)*}(R) O_R, \tag{2.73}$$

acts as a projection operator. Or in other words,

$$P_i^{(\mu)}\psi_j^{(\nu)} = \psi_i^{(\mu)}\delta_{ij}\delta_{\mu\nu}. \tag{2.74}$$

Let's try applying the projection operator to 2.67,

$$P_i^{(\mu)}\psi = \frac{n_\mu}{g}\sum_R D_{ii}^{(\mu)*}(R)O_R\psi = \frac{n_\mu}{g}\sum_R D_{ii}^{(\mu)*}(R)O_R\Big(\sum_\nu\sum_{j=1}^{n_\mu}\psi_i^{(\nu)}\Big) =$$
$$\sum_\nu\sum_{j=1}^{n_\mu}\frac{n_\mu}{g}\sum_R D_{ii}^{(\mu)*}(R)O_R\psi_j^{(\nu)} = \sum_\nu\sum_{j=1}^{n_\mu}P_i^{(\mu)}\psi_j^{(\nu)} = \sum_\nu\sum_{j=1}^{n_\mu}\psi_j^{(\mu)}\delta_{\mu\nu}\delta_{ij} = \psi_i^{(\mu)} \tag{2.75}$$

or

$$\psi_i^{(\mu)} = \frac{n_\mu}{g}\sum_R D_{ii}^{(\mu)*}(R)O_R\psi., \tag{2.76}$$

we say that a general function like ψ belongs to νth irreducible representation if it can be resolved in terms of its base functions. It is easy to show that all the theorems and lemmas that help us to derive the orthogonality relation for unitary representations is also valid for ray representations.

Considering an arbitrary function $g(r)$ like ψ, and a set of partner functions $f_n(\mathbf{r})$ like $\psi_i^{(\mu)}$, so we have,

$$f_0(\mathbf{r}) = \eta\sum_{\mathbf{R}_n} D_{11}^*(\mathbf{R}_n)T(\mathbf{R}_n)g(\mathbf{r}), \tag{2.77}$$

η is normalization coefficient and if we choose $\mathbf{R}_n$ to be $n\mathbf{a}_1$,

$$f_0(\mathbf{r}) = \eta\sum_{n=1}^{N} D_{11}^*(n\mathbf{a}_1)T(n\mathbf{a}_1)g(\mathbf{r}) = \eta\sum_{n=1}^{N}\delta_{11}\exp\Big(-i(1-1)\frac{2\pi ln}{N}\Big)T(n\mathbf{a}_1)g(\mathbf{r})$$
$$= \eta\sum_{n=1}^{N}T(n\mathbf{a}_1)g(\mathbf{r}). \tag{2.78}$$

The other element of the given representation can be taken as $-m\mathbf{a}_2$(we took negative for convenience). Hence, the other partner functions are related as the following:

$$T(-m\mathbf{a}_2)f_n(\mathbf{r}) = \sum_j D_{j+1,n+1}(-m\mathbf{a}_2)f_j(\mathbf{r})$$
$$= \sum_j \delta_{j+1,n+m+1}\, f_j(\mathbf{r}) = f_{n+m}(\mathbf{r}) \tag{2.79}$$
$$\Rightarrow T(-m\mathbf{a}_2)f_n(\mathbf{r}) = f_{n+m}(\mathbf{r})$$

and

$$
\begin{aligned}
T(\mathbf{a}_1)f_n(\mathbf{r}) &= \sum_j D_{j+1,n+1}(\mathbf{a}_1)f_j(\mathbf{r}) \\
&= \sum_j \delta_{j+1,n+1} \exp\Big(ij\frac{2\pi l}{N}\Big) f_j(\mathbf{r}) = \exp\Big(in\frac{2\pi l}{N}\Big) f_n(\mathbf{r}) \\
&\Rightarrow T(\mathbf{a}_1)f_n(\mathbf{r}) = \exp\Big(in\frac{2\pi l}{N}\Big) f_n(\mathbf{r}).
\end{aligned} \tag{2.80}
$$

It is appropriate now to investigate a crystal with bigger dimensions undergoing magnetically periodic boundary conditions. The dimensions are $N_1\mathbf{a}_1$, $N_2\mathbf{a}_2$, $N_3\mathbf{a}_3$ where $N_1 = M_1N$, $N_2 = M_2N$ and the magnetic field is chosen in direction of $\mathbf{a}_3$ as before. We have a larger group, with $N_1N_2N_3$ number of operations. The number of representations are $M_1M_2N_3$ with dimensionality N for discussed group G. The matrices that we are dealing here are assigned with reciprocal space components of $\mathbf{q}_1$, $\mathbf{q}_2$, $\mathbf{q}_3$ differing with real space translation matrices that we have worked before by a phase factor,

$$
D^q(\mathbf{a}_j) = \exp(-i\mathbf{q}_j\mathbf{a}_j)D(\mathbf{a}_j) \quad j = 1, 2, 3. \tag{2.81}
$$

We take both sides of equation 2.81 to power of N_j,

$$
\begin{aligned}
&\big[D^q(\mathbf{a}_j)\big]^{N_j} = \big[\exp(-i\mathbf{q}_j\mathbf{a}_j)D(\mathbf{a}_j)\big]^{N_j} \\
&\Rightarrow \big[D^q(\mathbf{a}_j)\big]^{N_j} = \exp(-i\mathbf{q}_j\mathbf{a}_jN_j)\big[D(\mathbf{a}_j)\big]^{N_j} \\
&\Rightarrow 1 = \exp(-i\mathbf{q}_j\mathbf{a}_jN_j) \times 1 \\
&\Rightarrow \exp(-i\mathbf{q}_j\mathbf{a}_jN_j) = 1
\end{aligned} \tag{2.82}
$$

$$
\begin{aligned}
&\mathbf{q}_j\mathbf{a}_jN_j = 2\pi C_j \quad j = 1, 2, 3 \\
&C_1 = 0, 1, \ldots, M_1 - 1;\ C_2 = 0, 1, \ldots, M_2 - 1 \\
&C_3 = 0, 1, \ldots, N_3 - 1.
\end{aligned} \tag{2.83}
$$

Let's remind equation 2.76,

$$\psi_i^{(\mu)} = \frac{n_\mu}{g} \sum_R D_{ii}^{(\mu)*}(R) O_R \psi,$$

if elements R, S, and T belong to group G, then we can replace R with RST and it will also sum on all over elements of G,

$$\begin{aligned}
\psi_i^{(\mu)} &= \frac{n_\mu}{g} \sum_{RST} D_{ii}^{(\mu)*}(RST) O_{RST} \psi \\
&= \frac{n_\mu}{g} \sum_{R,S,T} D_{ii}^{(\mu)*}(R) D_{ii}^{(\mu)*}(S) D_{ii}^{(\mu)*}(T) O_R O_S O_T \psi \\
&= \frac{n_\mu}{g} \sum_R D_{ii}^{(\mu)*}(R) O_R \sum_S D_{ii}^{(\mu)*}(S) O_S \sum_T D_{ii}^{(\mu)*}(T) O_T \psi,
\end{aligned} \tag{2.84}$$

If we replace as following,

$$\begin{aligned}
&\frac{n_\mu}{g} \to \eta && R \to n_1 \mathbf{a}_1 && \psi \to g(\mathbf{r}) \\
&S \to n_3 \mathbf{a}_3 && T \to n_2 N \mathbf{a}_2 && \psi_i^{(\mu)} \to f_0^q(\mathbf{r})
\end{aligned} \tag{2.85}$$

then

$$f_0^q(\mathbf{r}) = \eta \sum_{n_1}^{N_1} D_{ii}^{q*}(n_1 \mathbf{a}_1) T(n_1 \mathbf{a}_1) \sum_{n_2}^{N_2} D_{ii}^{q*}(n_2 N \mathbf{a}_2) T(n_2 N \mathbf{a}_2) \sum_{n_3}^{N_3} D_{ii}^{q*}(n_3 \mathbf{a}_3) T(n_3 \mathbf{a}_3) g(r),$$

$$\begin{aligned}
\Rightarrow f_0^q(\mathbf{r}) =& \eta \sum_{n_1=1}^{N_1} \exp(i q_1 n_1 a_1) D_{11}(n_1 \mathbf{a}_1) T(n_1 \mathbf{a}_1) \sum_{n_2=1}^{N_2} \exp(i q_2 n_2 N a_2) D_{11}(n_2 N \mathbf{a}_2) T(n_2 N \mathbf{a}_2) \\
& \sum_{n_3=1}^{N_3} \exp(i q_3 n_3 a_3) D_{11}(n_3 \mathbf{a}_3) T(n_3 \mathbf{a}_3) g(\mathbf{r}) = \\
& \eta \sum_{n_1, n_2, n_3} \exp[i(q_1 n_1 a_1 + q_2 n_2 N a_2 + q_3 n_3 a_3)] \\
& \qquad \times T(n_1 \mathbf{a}_1) T(n_2 N \mathbf{a}_2) T(n_3 \mathbf{a}_3) g(\mathbf{r}),
\end{aligned} \tag{2.86}$$

where is generalization of a Bloch sum. Using equation 2.32, we can find a similar equation as 2.79 for $f^q(\mathbf{r})$:

$$T(-m\mathbf{a}_2)f_0^q(\mathbf{r}) = \sum_l D^q_{l+1,0+1}(-m\mathbf{a}_2)f_l^q(\mathbf{r}) = \sum_l \exp(iq_2ma_2)D_{l+1,0+1}(-m\mathbf{a}_2)f_l^q(\mathbf{r})$$
$$= \sum_l \exp(iq_2ma_2)\delta_{l+1,m+1}f_l^q(\mathbf{r}) = \exp(iq_2ma_2)f_m^q(\mathbf{r}),$$

$$\Rightarrow f_m^q(\mathbf{r}) = \exp(-iq_2ma_2)T(-m\mathbf{a}_2)f_0^q(\mathbf{r}). \tag{2.87}$$

This relation can be generalized to a vector constructed by $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$:

$$\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3, \tag{2.88}$$

it will be,

$$\begin{aligned} &T(-\mathbf{R}_n)f_m^q(\mathbf{r}) = T(-n_1\mathbf{a}_1 - n_2\mathbf{a}_2 - n_3\mathbf{a}_3)f_m^q(\mathbf{r}) = \\ &T(-n_1\mathbf{a}_1 - n_2\mathbf{a}_2)T(-n_3\mathbf{a}_3)\exp\Big[(i/2)\big[(-n_1\mathbf{a}_1 - n_2\mathbf{a}_2)\times(-n_3\mathbf{a}_3)\big]\cdot\boldsymbol{\beta}\Big]f_m^q(\mathbf{r}) = \\ &T(-n_1\mathbf{a}_1 - n_2\mathbf{a}_2)T(-n_3\mathbf{a}_3)f_m^q(\mathbf{r}), \end{aligned} \tag{2.89}$$

then

$$\begin{aligned} &T(-n_1\mathbf{a}_1 - n_2\mathbf{a}_2)T(-n_3\mathbf{a}_3)f_m^q(\mathbf{r}) = \\ &T(-n_1\mathbf{a}_1)T(-n_2\mathbf{a}_2)T(-n_3\mathbf{a}_3)\exp\Big[(i/2)\big[(-n_1\mathbf{a}_1)\times(-n_2\mathbf{a}_2)\big]\cdot\boldsymbol{\beta}\Big]f_m^q(\mathbf{r}) = \\ &T(-n_1\mathbf{a}_1)T(-n_2\mathbf{a}_2)T(-n_3\mathbf{a}_3)\exp\Big[(i/2)(n_1n_2)\big[(\mathbf{a}_2\times\boldsymbol{\beta})\big]\cdot\mathbf{a}_1\Big]f_m^q(\mathbf{r}) = \\ &T(-n_1\mathbf{a}_1)T(-n_2\mathbf{a}_2)T(-n_3\mathbf{a}_3)\exp\Big[(i/2)(n_2)\big[(\mathbf{a}_2\times\boldsymbol{\beta})\big]\cdot(n_1\mathbf{a}_1)\Big]f_m^q(\mathbf{r}) = \\ &T(-n_1\mathbf{a}_1)T(-n_2\mathbf{a}_2)T(-n_3\mathbf{a}_3)\exp\Big[(i/2)(n_2)\big[(\mathbf{a}_2\times\boldsymbol{\beta})\big]\cdot(\mathbf{R}_n)\Big]f_m^q(\mathbf{r}) = \\ &T(-n_1\mathbf{a}_1)T(-n_2\mathbf{a}_2)T(-n_3\mathbf{a}_3)\exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big]f_m^q(\mathbf{r}), \end{aligned} \tag{2.90}$$

$$
\begin{aligned}
&\Rightarrow T(-\mathbf{R}_n) f_m^q(\mathbf{r}) = \\
&\quad T(-n_1\mathbf{a}_1)T(-n_2\mathbf{a}_2)T(-n_3\mathbf{a}_3)\exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big] f_m^q(\mathbf{r}) = \\
&\quad \exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big] T(-n_1\mathbf{a}_1)T(-n_2\mathbf{a}_2)T(-n_3\mathbf{a}_3) f_m^q(\mathbf{r}) = \\
&\quad \exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big] T(-n_1\mathbf{a}_1)T(-n_2\mathbf{a}_2)\Big\{T(-n_3\mathbf{a}_3) f_m^q(\mathbf{r})\Big\} = \\
&\quad \exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big] T(-n_1\mathbf{a}_1)T(-n_2\mathbf{a}_2) \\
&\quad \Big\{\sum_p D^q_{p+1,m+1}(-n_3\mathbf{a}_3) f_p^q(\mathbf{r})\Big\} = \\
&\quad \exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big] T(-n_1\mathbf{a}_1)T(-n_2\mathbf{a}_2) \\
&\quad \Big\{\sum_p \exp(iq_3n_3\mathbf{a}_3) D_{p+1,m+1}(-n_3\mathbf{a}_3) f_p^q(\mathbf{r})\Big\} = \\
&\quad \exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big] \exp(iq_3n_3\mathbf{a}_3) T(-n_1\mathbf{a}_1)T(-n_2\mathbf{a}_2) \\
&\quad \Big\{\sum_p \delta_{p+1,m+1} f_p^q(\mathbf{r})\Big\} = \\
&\quad \exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big] \exp(iq_3n_3\mathbf{a}_3) T(-n_1\mathbf{a}_1)T(-n_2\mathbf{a}_2) \\
&\quad \Big\{f_m^q(\mathbf{r})\Big\} = \\
&\quad \exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big] \exp(iq_3n_3\mathbf{a}_3) T(-n_1\mathbf{a}_1) \\
&\quad \Big\{T(-n_2\mathbf{a}_2) f_m^q(\mathbf{r})\Big\} =
\end{aligned}
\tag{2.91}
$$

$$
\begin{aligned}
&\exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big]\exp(iq_3n_3\mathbf{a}_3)T(-n_1\mathbf{a}_1)\\
&\Big\{\sum_p D^q_{p+1,m+1}(-n_2\mathbf{a}_2)f^q_p(\mathbf{r})\Big\}=\\
&\exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big]\exp(iq_3n_3\mathbf{a}_3)T(-n_1\mathbf{a}_1)\\
&\Big\{\sum_p \exp(iq_2n_2\mathbf{a}_2)D^q_{p+1,m+1}(-n_2\mathbf{a}_2)f^q_p(\mathbf{r})\Big\}=\\
&\exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big]\exp(iq_3n_3\mathbf{a}_3)\exp(iq_2n_2\mathbf{a}_2)T(-n_1\mathbf{a}_1)\\
&\Big\{\sum_p \delta^q_{p+1,m+1+n_2}f^q_p(\mathbf{r})\Big\}=\\
&\exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big]\exp(iq_3n_3\mathbf{a}_3)\exp(iq_2n_2\mathbf{a}_2)T(-n_1\mathbf{a}_1)\\
&\Big\{f^q_{m+n_2}(\mathbf{r})\Big\}=\\
&\exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big]\exp(iq_3n_3\mathbf{a}_3)\exp(iq_2n_2\mathbf{a}_2)\\
&\Big\{T(-n_1\mathbf{a}_1)f^q_{m+n_2}(\mathbf{r})\Big\}=\\
&\exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big]\exp(iq_3n_3\mathbf{a}_3)\exp(iq_2n_2\mathbf{a}_2)\\
&\Big\{\sum_p D^q_{p+1,m+n_2+1}(-n_1\mathbf{a}_1)f^q_p(\mathbf{r})\Big\}=\\
&\exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big]\exp(iq_3n_3\mathbf{a}_3)\exp(iq_2n_2\mathbf{a}_2)\\
&\Big\{\sum_p \exp(iq_1n_1\mathbf{a}_1)D_{p+1,m+n_2+1}(-n_1\mathbf{a}_1)f^q_p(\mathbf{r})\Big\}=\\
&\exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big]\exp(iq_3n_3\mathbf{a}_3)\exp(iq_2n_2\mathbf{a}_2)\exp(iq_1n_1\mathbf{a}_1)\\
&\Big\{\sum_p \delta_{p+1,m+n_2+1}\exp(-ip2\pi ln_1/N)f^q_p(\mathbf{r})\Big\}=\\
&\exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot(\mathbf{R}_n)\Big]\exp(iq_3n_3\mathbf{a}_3)\exp(iq_2n_2\mathbf{a}_2)\exp(iq_1n_1\mathbf{a}_1)\\
&\Big\{\exp\big[-i(m+n_2)2\pi ln_1/N\big]f^q_{m+n_2}(\mathbf{r})\Big\},
\end{aligned}
\tag{2.92}
$$

since we know that,

$$(\boldsymbol{\beta}\times\mathbf{a}_2)\cdot\mathbf{R}_1=(\frac{2\pi l}{\Omega N}\mathbf{a}_3\times\mathbf{a}_2)\cdot(n_1\mathbf{a}_1)=\frac{2\pi l n_1}{\Omega N}(\mathbf{a}_3\times\mathbf{a}_2)\cdot\mathbf{a}_1=\\ \frac{2\pi l n_1}{\Omega N}(\mathbf{a}_3\times\mathbf{a}_2)\cdot\mathbf{a}_1=\frac{2\pi l n_1}{\Omega N}(-\Omega)=\frac{-2\pi l n_1}{N}, \tag{2.93}$$

so we can replace $(-2\pi l n_1)/N$ with $(\boldsymbol{\beta}\times\mathbf{a}_2)\cdot\mathbf{R}_n$,

$$\begin{aligned}
&\Rightarrow T(-\mathbf{R}_n)f^q_m(\mathbf{r})=\\
&\exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\cdot\mathbf{R}_n\big]\Big]\exp\Big[i(m+n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\cdot\mathbf{R}_n\big]\Big]\\
&\exp(iq_3n_3\mathbf{a}_3)\exp(iq_2n_2\mathbf{a}_2)\exp(iq_1n_1\mathbf{a}_1)\Big\{f^q_{m+n_2}(\mathbf{r})\Big\}=\\
&\exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\cdot\mathbf{R}_n\big]\Big]\exp\Big[i(m+n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\cdot\mathbf{R}_n\big]\Big]\\
&\exp(iq_3n_3\mathbf{a}_3+iq_2n_2\mathbf{a}_2+iq_1n_1\mathbf{a}_1)\Big\{f^q_{m+n_2}(\mathbf{r})\Big\}=\\
&\exp\Big[(-i/2)(n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\cdot\mathbf{R}_n\big]\Big]\exp\Big[i(m+n_2)\big[(\boldsymbol{\beta}\times\mathbf{a}_2)\cdot\mathbf{R}_n\big]\Big]\\
&\exp(i\mathbf{q}\cdot\mathbf{R}_n)\Big\{f^q_{m+n_2}(\mathbf{r})\Big\}=\\
&\exp\Big[(i\big[\mathbf{q}+(m+n_2/2)(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot\mathbf{R}_n)\Big]\Big\{f^q_{m+n_2}(\mathbf{r})\Big\},
\end{aligned} \tag{2.94}$$

or

$$T(-\mathbf{R}_n)f^q_m(\mathbf{r})=\exp\Big[(i\big[\mathbf{q}+(m+n_2/2)(\boldsymbol{\beta}\times\mathbf{a}_2)\big]\cdot\mathbf{R}_n)\Big]f^q_{m+n_2}(\mathbf{r}). \tag{2.95}$$

This equation uncovers how the basis of the irreducible representation is transforming. To show the resemblance of the obtained equation with usual Bloch functions, we can replace

$$B(\mathbf{r};\mathbf{q}+m\boldsymbol{\beta}\times\mathbf{a}_2)=f^q_m(\mathbf{r}) \tag{2.96}$$

or in another words,

$$T(-\mathbf{R}_n)B(\mathbf{r};\mathbf{k})=\exp\Big[(i\big[\mathbf{k}+\boldsymbol{\beta}\times n_2\mathbf{a}_2/2)\big]\cdot\mathbf{R}_n)\Big]B(\mathbf{r};\mathbf{k}+\boldsymbol{\beta}\times n_2\mathbf{a}_2). \tag{2.97}$$

2.2 Magnetic translation operators

The modified translation operators introduced by E. Brown [1] forms ray group. J.Zak [2] defined a new set of translation operators where it combines the ordinary translation operator with a new part depending on the path that connects a point to another. These new set of translation operators are called magnetic translation operators where form a full group rather than ray group. Let's consider the Hamiltonian of a Bloch electron in a magnetic field with the same gauge for the vector potential that we considered at beginning of this chapter.

$$H = \frac{1}{2m}\left(\mathbf{p} + \frac{e\mathbf{A}}{c}\right)^2 + V(\mathbf{r}) \tag{2.98}$$

with the gauge:

$$\mathbf{A} = \frac{1}{2}(\mathbf{H} \times \mathbf{r}) \tag{2.99}$$

where $\mathbf{H}$ is the magnetic field. Let's consider a Bravais lattice:

$$\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \tag{2.100}$$

where $\{\mathbf{a}_i\}$ are primitive vectors. Let assume we have a path connecting point O to the point defined by $\mathbf{R}_n$ and we can travel from one lattice point to another by using Bravais lattice vectors. We can consider a path as following:

$$\mathbf{R}_n = \mathbf{R}_1 + \mathbf{R}_2 + \ldots + \mathbf{R}_i, \tag{2.101}$$

and we can demonstrate the path as:

$$|\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_i). \tag{2.102}$$

It is easy to see that this path is not unique and one can have many other paths satisfying equation 2.101. The new operator which is combination of modified translation operator and one extra part can be written as:

$$\begin{aligned}\tau(\mathbf{R}_n|\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_i) = &\exp\left\{(i/\hbar)\mathbf{R}_n \cdot [\mathbf{p} - (e/c)\mathbf{A}]\right\} \\ &\times \exp\left\{(i/2)[\mathbf{R}_1 \times \mathbf{R}_2 + \mathbf{R}_1 \times \mathbf{R}_3 + \ldots + \mathbf{R}_{i-1} \times \mathbf{R}_i] \cdot \mathbf{h}\right\}\end{aligned} \tag{2.103}$$

where $\mathbf{h} = e\mathbf{H}/\hbar c$. The vector products of $\{\mathbf{R}_j\}_{j=1}^{i}$ have the same order given by the path that they are forming. We can see that,

$$\frac{1}{2}[\mathbf{R}_1 \times \mathbf{R}_2 + \mathbf{R}_1 \times \mathbf{R}_3 + \ldots + \mathbf{R}_{i-1} \times \mathbf{R}_i] \cdot \mathbf{h} \tag{2.104}$$

have a simple meaning. If we project each $\mathbf{R}_j$ to the plane in which the normal vector is $\hat{\mathbf{h}}$ where it is the unit vector along the vector $\mathbf{h}$, then the path projection on the plane is given by,

$$|\mathbf{R}_1^p, \mathbf{R}_2^p, \ldots, \mathbf{R}_i^p) \tag{2.105}$$

and it is not hard to see that,

$$\begin{aligned} &\frac{1}{2}[\mathbf{R}_1 \times \mathbf{R}_2 + \mathbf{R}_1 \times \mathbf{R}_3 + \ldots + \mathbf{R}_{i-1} \times \mathbf{R}_i] \cdot \mathbf{h} \\ &\qquad = \frac{1}{2}[\mathbf{R}_1^p \times \mathbf{R}_2^p + \mathbf{R}_1 \times \mathbf{R}_3^p + \ldots + \mathbf{R}_{i-1}^p \times \mathbf{R}_i^p] \cdot \mathbf{h}. \end{aligned} \tag{2.106}$$

Here the right-hand-side of equation 2.106 is the area that is embodied by the projected vectors:

$$\mathbf{R}_1^p, \mathbf{R}_2^p, \ldots, \mathbf{R}_i^p, -\mathbf{R}_n^p \tag{2.107}$$

the vector $-\mathbf{R}_n^p$ helps to close the path. These vectors construct a polygon and the expression 2.104 is the flux passing through the embodied area by the polygon,

$$\begin{aligned} \tau(\mathbf{R}_n|\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_i) = &\exp\left\{(i/\hbar)\mathbf{R}_n \cdot [\mathbf{p} - (e/c)\mathbf{A}]\right\} \\ &\times \exp\left\{i\phi(\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_i)\right\}. \end{aligned} \tag{2.108}$$

In order to check that the new defined operator is forming a full group or not, we will calculate the following:

$$\begin{aligned} &\tau(\mathbf{R}_n|\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_i)\tau(\mathbf{R}'_n|\mathbf{R}'_1, \mathbf{R}'_2, \ldots, \mathbf{R}'_k) \\ &= \exp\left\{(i/\hbar)\mathbf{R}_n \cdot [\mathbf{p} - (e/c)\mathbf{A}]\right\} \\ &\times \exp\left\{(i/2)[\mathbf{R}_1 \times \mathbf{R}_2 + \mathbf{R}_1 \times \mathbf{R}_3 + \ldots + \mathbf{R}_{i-1} \times \mathbf{R}_i] \cdot \mathbf{h}\right\} \\ &\times \exp\left\{(i/\hbar)\mathbf{R}'_n \cdot [\mathbf{p} - (e/c)\mathbf{A}]\right\} \\ &\times \exp\left\{(i/2)[\mathbf{R}'_1 \times \mathbf{R}'_2 + \mathbf{R}'_1 \times \mathbf{R}'_3 + \ldots + \mathbf{R}'_{k-1} \times \mathbf{R}'_k] \cdot \mathbf{h}\right\} \\ &= \exp\left\{(i/\hbar)\mathbf{R}_n \cdot [\mathbf{p} - (e/c)\mathbf{A}]\right\} \\ &\times \exp\left\{(i/\hbar)\mathbf{R}'_n \cdot [\mathbf{p} - (e/c)\mathbf{A}]\right\} \\ &\times \exp\left\{(i/2)[\mathbf{R}_1 \times \mathbf{R}_2 + \mathbf{R}_1 \times \mathbf{R}_3 + \ldots + \mathbf{R}_{i-1} \times \mathbf{R}_i \right. \\ &\left. + \mathbf{R}'_1 \times \mathbf{R}'_2 + \mathbf{R}'_1 \times \mathbf{R}'_3 + \ldots + \mathbf{R}'_{k-1} \times \mathbf{R}'_k] \cdot \mathbf{h}\right\}, \end{aligned} \tag{2.109}$$

Baker-Campbell-Hausdorff formula is given by:

$$\exp(A)\exp(B) = \exp(A + B + \frac{1}{2}[A, B]) \tag{2.110}$$

and it helps to calculate the following,

$$\Big[\frac{i}{\hbar}\mathbf{R}_n \cdot \Big(\mathbf{p} - \frac{e}{c}\mathbf{A}\Big), \frac{i}{\hbar}\mathbf{R}'_n \cdot \Big(\mathbf{p} - \frac{e}{c}\mathbf{A}\Big)\Big] = i(\mathbf{R}_n \times \mathbf{R}'_n) \cdot \mathbf{h} \tag{2.111}$$

therefore,

$$\begin{aligned}
&\tau(\mathbf{R}_n|\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_i)\tau(\mathbf{R}'_n|\mathbf{R}'_1, \mathbf{R}'_2, \ldots, \mathbf{R}'_k) \\
&= \exp\big\{(i/\hbar)(\mathbf{R}_n + \mathbf{R}'_n) \cdot [\mathbf{p} - (e/c)\mathbf{A}]\big\} \\
&\times \exp\big\{(i/2)[\mathbf{R}_1 \times \mathbf{R}_2 + \ldots + \mathbf{R}_1 \times \mathbf{R}'_1 + \ldots \\
&+ \mathbf{R}'_{k-1} \times \mathbf{R}'_k] \cdot \mathbf{h}\big\}.
\end{aligned} \tag{2.112}$$

So the total path would be:

$$|\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_i, \mathbf{R}'_1, \mathbf{R}'_2, \ldots, \mathbf{R}'_k) \tag{2.113}$$

thus, the path 2.113 provides the following magnetic translation operator:

$$\begin{aligned}
&\tau(\mathbf{R}_n|\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_i)\tau(\mathbf{R}'_n|\mathbf{R}'_1, \mathbf{R}'_2, \ldots, \mathbf{R}'_k) \\
&= \tau(\mathbf{R}_n + \mathbf{R}'_n|\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_i, \mathbf{R}'_1, \mathbf{R}'_2, \ldots, \mathbf{R}'_k).
\end{aligned} \tag{2.114}$$

Equation 2.114 provides a full group. To investigate the group conditions first we need to consider the reciprocal operator $\tau(-\mathbf{R}_n| - \mathbf{R}_i, -\mathbf{R}_{i-1}, \ldots, -\mathbf{R}_1)$ which guarantees the existence of identity element for the group. Let us denote the current group as G. We can call this group as magnetic translation group(M.T.G). This is an infinite group for two reasons. There are infinite number of vectors $\mathbf{R}_n$ and for each vector there are infinite number of paths. We can introduce another group H in which each member like $H(\mathbf{R}_n)$ corresponds to elements of G given with vector $\mathbf{R}_n$ but with different paths. Therefore group G is homomorphic to H. The new defined group H is abelian group. It means that $H(\mathbf{R}_n + \mathbf{R}'_n) = H(\mathbf{R}'_n + \mathbf{R}_n)$. Since the group H is isomorphic to the usual translation group, denoted by R, hence there exist a homomorphism from G to R which helps to use the Born-von Karman boundary conditions to construct matrix representations for magnetic translation operators.

2.3 Translation operators in phase space

We learned about space translation and momentum translation operators in quantum mechanics textbook. We can define the translation operator in one-dimensional space coordinate as:

$$T(\Delta x) = \exp\Big[-i\frac{(\Delta x)p_x}{\hbar}\Big] \tag{2.115}$$

and translation operator in one-dimensional momentum coordinate as:

$$T(\Delta p_x) = \exp\Big[-i\frac{(\Delta p_x)x}{\hbar}\Big]. \tag{2.116}$$

We can define a new operator in the following form:

$$T(\Delta x^{(n)}, \Delta p_x^{(n)}) = \exp\Big[-i\frac{(\Delta x)^{(n)}p_x}{\hbar} - i\frac{(\Delta p_x)^{(n)}x}{\hbar}\Big], \tag{2.117}$$

and we denote the displacement in phase space coordinates with the vector $\mathbf{\Gamma}_n$:

$$\mathbf{\Gamma}_n = \begin{pmatrix}\Delta x^{(n)} \\ \Delta p_x^{(n)}\end{pmatrix} \tag{2.118}$$

Hence, it would be easier to express the new defined operator in terms of $\mathbf{\Gamma}_n$:

$$T(\Delta x^{(n)}, \Delta p_x^{(n)}) = T(\mathbf{\Gamma}_n) \tag{2.119}$$

then, we can find out whether new defined operator is forming a group or not.

$$\begin{aligned}
&T(\mathbf{\Gamma}_n)T(\mathbf{\Gamma}'_n) = \exp\Big\{-i\frac{(\Delta x^{(n)})p_x}{\hbar} - i\frac{(\Delta p_x^{(n)})x}{\hbar}\Big\}\exp\Big\{-i\frac{(\Delta x^{(n)\prime})p_x}{\hbar} - i\frac{(\Delta p_x^{(n)\prime})x}{\hbar}\Big\} \\
&= \exp\Big\{-i\frac{(\Delta x^{(n)})p_x}{\hbar} - i\frac{(\Delta p_x^{(n)})x}{\hbar} - i\frac{(\Delta x^{(n)\prime})p_x}{\hbar} - i\frac{(\Delta p_x^{(n)\prime})x}{\hbar}\Big\} \\
&\times \exp\Big\{\Big[-i\frac{(\Delta x^{(n)})p_x}{\hbar} - i\frac{(\Delta p_x^{(n)})x}{\hbar}\,,\, -i\frac{(\Delta x^{(n)\prime})p_x}{\hbar} - i\frac{(\Delta p_x^{(n)\prime})x}{\hbar}\Big]\Big\} \\
&= \exp\Big\{-i\frac{(\Delta x^{(n)} + \Delta x^{(n)\prime})p_x}{\hbar} - i\frac{(\Delta p_x^{(n)} + \Delta p_x^{(n)\prime})x}{\hbar}\Big\} \\
&\times \exp\Big\{\Big[-i\frac{(\Delta x^{(n)})p_x}{\hbar} - i\frac{(\Delta p_x^{(n)})x}{\hbar}\,,\, -i\frac{(\Delta x^{(n)\prime})p_x}{\hbar} - i\frac{(\Delta p_x^{(n)\prime})x}{\hbar}\Big]\Big\} \\
&= \exp\Big\{-i\frac{(\Delta x^{(n)} + \Delta x^{(n)\prime})p_x}{\hbar} - i\frac{(\Delta p_x^{(n)} + \Delta p_x^{(n)\prime})x}{\hbar}\Big\} \\
&\times \exp\Big\{\frac{i}{2\hbar}(\Delta x^{(n)}\Delta p_x^{(n)\prime} - \Delta p_x^{(n)}\Delta x^{(n)\prime})\Big\} \\
&= T(\mathbf{\Gamma}_n + \mathbf{\Gamma}'_n)\exp\Big\{\frac{i}{2\hbar}(\mathbf{\Gamma}_n \times \mathbf{\Gamma}'_n)\cdot\hat{\mathbf{z}}\Big\}.
\end{aligned} \tag{2.120}$$

We also can write:

$$T(\mathbf{\Gamma}_n)T(\mathbf{\Gamma}'_n) = T(\mathbf{\Gamma}'_n)T(\mathbf{\Gamma}_n)\exp\Big\{-\frac{i}{2\hbar}(\mathbf{\Gamma}'_n \times \mathbf{\Gamma}_n)\cdot\hat{\mathbf{z}}\Big\}\exp\Big\{\frac{i}{2\hbar}(\mathbf{\Gamma}_n \times \mathbf{\Gamma}'_n)\cdot\hat{\mathbf{z}}\Big\} = T(\mathbf{\Gamma}'_n)T(\mathbf{\Gamma}_n)\exp\Big\{\frac{i}{\hbar}(\mathbf{\Gamma}_n \times \mathbf{\Gamma}'_n)\cdot\hat{\mathbf{z}}\Big\} \tag{2.121}$$

It is easy to check that the operators $T(\mathbf{\Gamma}_n)$ for different values of $\mathbf{\Gamma}_n$ are forming ray groups. From what we learned, similar to J. Zak work, we can introduce a new operator τ based on the operator T,

$$\tau(\mathbf{\Gamma}_n|\mathbf{\Gamma}_1, \mathbf{\Gamma}_2, \ldots, \mathbf{\Gamma}_i) \tag{2.122}$$

where $\mathbf{\Gamma}_n = \mathbf{\Gamma}_1 + \mathbf{\Gamma}_2 + \ldots + \mathbf{\Gamma}_i$.

$$|\mathbf{\Gamma}_1, \mathbf{\Gamma}_2, \ldots, \mathbf{\Gamma}_i) \tag{2.123}$$

denotes the path that connects point O to the point that the vector $\mathbf{\Gamma}_n$ is pointing. The new operator is expressible as:

$$\begin{aligned}\tau(\mathbf{\Gamma}_n|\mathbf{\Gamma}_1, \mathbf{\Gamma}_2, \ldots, \mathbf{\Gamma}_i) &= \exp\Big\{-i\frac{(\Delta x^{(n)})p_x}{\hbar} - i\frac{(\Delta p_x^{(n)})x}{\hbar}\Big\} \\ &\times \exp\Big\{\frac{i}{2\hbar}(\mathbf{\Gamma}_1 \times \mathbf{\Gamma}_2 + \mathbf{\Gamma}_1 \times \mathbf{\Gamma}_3 + \ldots + \mathbf{\Gamma}_{i-1} \times \mathbf{\Gamma}_i)\cdot\hat{\mathbf{z}}\Big\}\end{aligned} \tag{2.124}$$

where it forms a full group similar to 2.114,

$$\begin{aligned}\Rightarrow &\tau(\mathbf{\Gamma}_n|\mathbf{\Gamma}_1, \mathbf{\Gamma}_2, \ldots, \mathbf{\Gamma}_i)\tau(\mathbf{\Gamma}'_n|\mathbf{\Gamma}'_1, \mathbf{\Gamma}'_2, \ldots, \mathbf{\Gamma}'_k) \\ &= \tau(\mathbf{\Gamma}_n + \mathbf{\Gamma}'_n|\mathbf{\Gamma}_1, \mathbf{\Gamma}_2, \ldots, \mathbf{\Gamma}_i, \mathbf{\Gamma}'_1, \mathbf{\Gamma}'_2, \ldots, \mathbf{\Gamma}'_k).\end{aligned} \tag{2.125}$$

The group that is generated by translation operators τ holds the same properties that we discussed earlier at section 2.2. Although this group is not a symmetry group of a Hamiltonian with one dimensional potential given in the following form,

$$H = \frac{p^2}{2m} + v(x), \tag{2.126}$$

we still expect that by writing the Hamiltonian for specific cases of momentum and potential, we can find a Hamiltonian which commutes with the operator τ and provides the eigenvectors that matrix representations can be constructed based on them.

Chapter 3

Shifted Creutz model

Through this chapter, we are going to derive a toy model from Cruetz model while the band structure is shifted in k-space. This new model is one dimensional analog of Haldane model [3] in which the gaps can be opened and closed by manipulating the hopping terms at certain points. We adopt spin-orbit interaction to our model in a similar way that Kane-Mele [5] adopted the Haldane model. Shifted Creutz model breaks time-reversal symmetry while it holds a chiral symmetry. Unlike the spinless electrons model, in the shifted Creutz model with spin-orbit coupling, time-reversal symmetry appears and it is preserved.

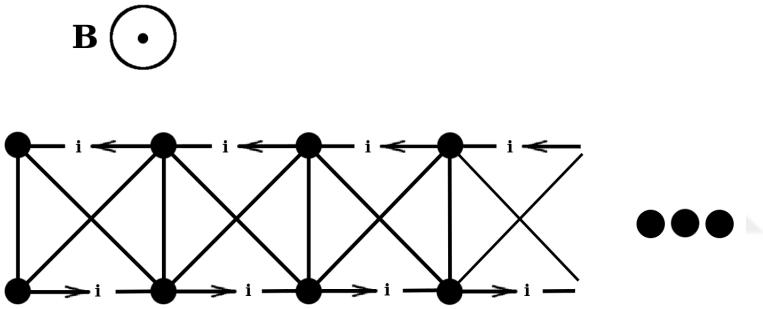
3.1 Creutz model

Creutz model [6] is given by a cross-linked ladder with spinless electrons in which the horizontal bonds is given by hopping parameter t_x. For diagonal and vertical bonds, the coupling is t_{xy} and t_y respectively. All these parameters are assumed

to be positive. The Hamiltonian of the model is,

$$\begin{aligned} H = -\sum_n [t_x(a_n^\dagger a_{n+1} \quad + \quad a_{n+1}^\dagger a_n \quad + \quad b_n^\dagger b_{n+1} \quad + \quad b_{n+1}^\dagger b_n) \\ + \quad t_{xy}(a_n^\dagger b_{n+1} \quad + \quad b_{n+1}^\dagger a_n \quad + \quad b_n^\dagger a_{n+1} \quad + \quad a_{n+1}^\dagger b_n) \\ + \quad t_y(a_n^\dagger b_n \quad + \quad b_n^\dagger a_n)]. \end{aligned} \tag{3.1}$$

where the fermionic annihilation and creation operators on the nth site of upper and lower chains are given by a_n, b_n and $a_n^\dagger$, $b_n^\dagger$, respectively. If we apply a magnetic field normal to the plane of the ladder, when an electron is hoping horizontally from one chain to another, it will be associated with a phase.



The new Hamiltonian is given in the form,

$$\begin{aligned} H = -\sum_n [t_x(e^{i\theta} a_n^\dagger a_{n+1} \quad + \quad e^{-i\theta} a_{n+1}^\dagger a_n \quad + \quad e^{-i\theta} b_n^\dagger b_{n+1} \quad + e^{i\theta} \quad b_{n+1}^\dagger b_n) \\ + \quad t_{xy}(a_n^\dagger b_{n+1} \quad + \quad b_{n+1}^\dagger a_n \quad + \quad b_n^\dagger a_{n+1} \quad + \quad a_{n+1}^\dagger b_n) \\ + \quad t_y(a_n^\dagger b_n \quad + \quad b_n^\dagger a_n)]. \end{aligned} \tag{3.2}$$

We can use Fourier transform and express our Hamiltonian in k-space,

$$H = -\int_0^{2\pi} \frac{dk}{2\pi} (a_k^\dagger \quad b_k^\dagger) \begin{pmatrix} 2t_x \cos(k-\theta) & t_y + 2t_{xy}\cos(k) \\ t_y + 2t_{xy}\cos(k) & 2t_x \cos(k+\theta) \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \tag{3.3}$$

where Fourier transform of annihilation and creation operators are given by,

$$\begin{aligned} a_n &= \frac{1}{\sqrt{N}} \sum_k a_k e^{-i\mathbf{k}.\mathbf{r}_n} & a_{n+1} &= \frac{1}{\sqrt{N}} \sum_k a_k e^{-i\mathbf{k}.(\mathbf{r}_n+\mathbf{1})} \\ b_n &= \frac{1}{\sqrt{N}} \sum_k b_k e^{-i\mathbf{k}.\mathbf{r}_n} & b_{n+1} &= \frac{1}{\sqrt{N}} \sum_k b_k e^{-i\mathbf{k}.(\mathbf{r}_n+\mathbf{1})} \end{aligned} \tag{3.4}$$

and energy eigenvalues at $\theta = \pi/2$ are:

$$E(k) = \pm\sqrt{(2t_x \sin(k))^2 + (t_y + 2t_{xy}\cos(k))^2}. \tag{3.5}$$

If we set $t_y - 2t_{xy} = 0$, in the band structure, there exist gap closure at points $k = -\pi$ and $k = \pi$ with 0 energies and they are called time reversal invariant momenta.

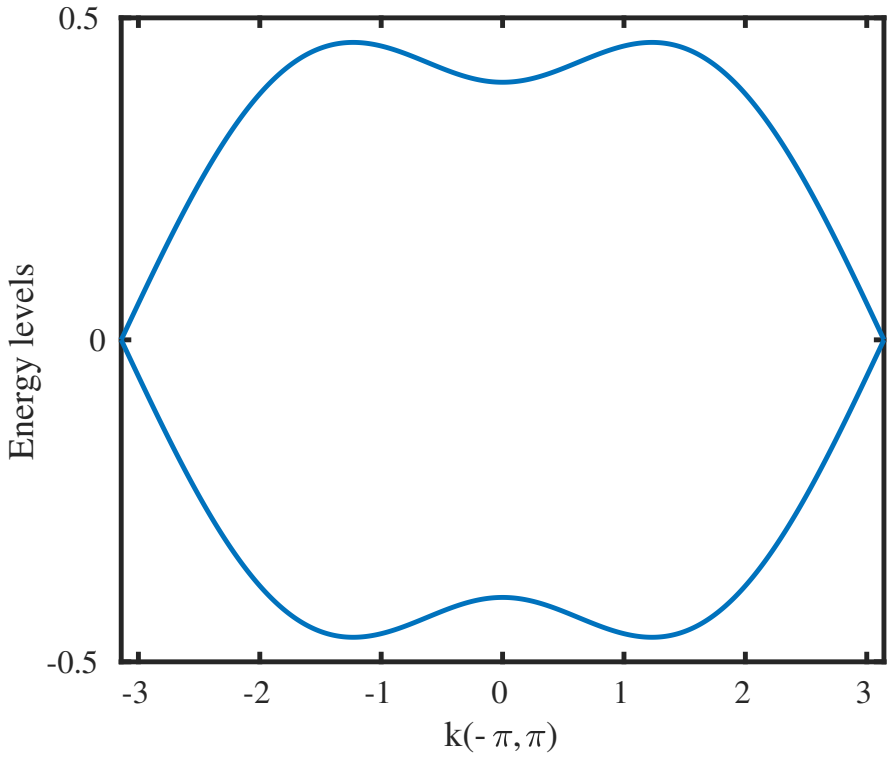


Figure 3.1: Band structure of Creutz model; The values are set as $t_x = 0.2$, $t_{xy} = 0.1$, and $t_y = 0.2$ in a periodic boundary condition.

3.2 Shifted Creutz model

We shift Creutz model in k-axis for $\pi/2$. New shifted band structure in contrast to Creutz model loses the time reversal symmetry and it only shows one gap closure at $k = \pi/2$.

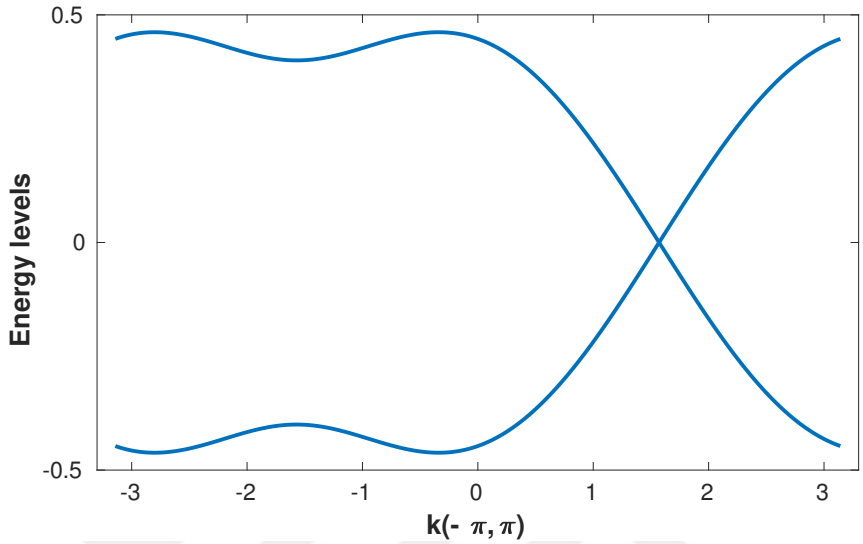
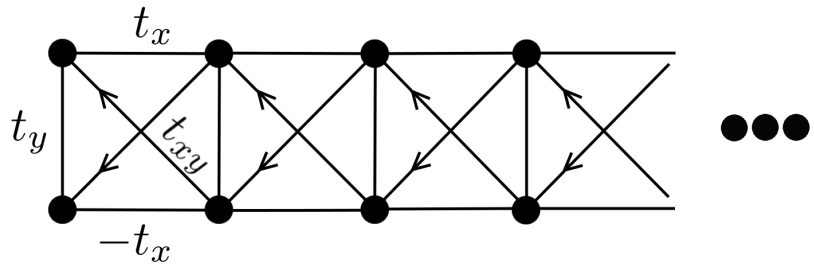


Figure 3.2: Band structure of shifted Creutz model; The values are set as $t_x = 0.2$, $t_{xy} = 0.1$, and $t_y = 0.2$ in a periodic boundary condition.

A cross-linked ladder similar to Creutz-model with phases on diagonal bonds while the hopping term for horizontal bonds in upper chains is t_x and for lower chains is $-t_x$ is providing us the same band structure and it can be depicted as:



The structure is considered again as spinless electrons. Let's assume that introduced parameters are positive same as Creutz. The shifted Creutz Hamiltonian can be written as following:

$$
\begin{aligned}
H = -\sum_{n} \\
&[t_x(a_n^\dagger a_{n+1} \quad + \quad a_{n+1}^\dagger a_n) \quad - \quad t_x(b_n^\dagger b_{n+1} \quad + \quad b_{n+1}^\dagger b_n) \\
&+ t_{xy}(e^{-i\theta} a_n^\dagger b_{n+1} \quad + \quad e^{+i\theta} b_{n+1}^\dagger a_n \quad + \quad e^{-i\theta} b_n^\dagger a_{n+1} \quad + \quad e^{+i\theta} a_{n+1}^\dagger b_n) \\
&+ t_y(a_n^\dagger b_n \quad + \quad b_n^\dagger a_n)].
\end{aligned}
\tag{3.6}
$$

We can use Fourier transform given by 3.4 and express our Hamiltonian in k-space with particular magnetic flux $\theta = \pi/2$,

$$
H = -\int_0^{2\pi} \frac{dk}{2\pi} (a_k^\dagger \quad b_k^\dagger) \begin{pmatrix} 2t_x \cos(k) & t_y - 2t_{xy} \sin(k) \\ t_y - 2t_{xy} \sin(k) & -2t_x \cos(k) \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \tag{3.7}
$$

and this time the energy eigenvalues are:

$$
E(k) = \pm\sqrt{(2t_x \cos(k))^2 + (t_y - 2t_{xy} \sin(k))^2}. \tag{3.8}
$$

If we set $t_y = 2t_{xy}$, there would be a degenerate state at the point $k = \pi/2$, while it would be gapless in other points of Brillouin zone(Fig. 3.2).

3.2.1 Winding Number

In mathematics, winding number measures the number of times that a curve wraps a given point. Winding number is a good mathematical geometric quantity to characterize the topological properties of phase transition points at 1D systems. It reveals the topological properties of the system by getting determined as a topological invariant on closed curves surrounding the transition points. Let us consider the 1D shifted-Creutz model once again and calculate the winding number:

$$
H = -\int_0^{2\pi} \frac{dk}{2\pi} (a_k^\dagger \quad b_k^\dagger) \begin{pmatrix} 2t_x \cos(k) & t_y - 2t_{xy} \sin(k) \\ t_y - 2t_{xy} \sin(k) & -2t_x \cos(k) \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \tag{3.9}
$$

The kernel of Hamiltonian can be written in term of Pauli matrices,

$$\mathcal{H}(k) = \begin{pmatrix} 2t_x\cos(k) & t_y - 2t_{xy}\sin(k) \\ t_y - 2t_{xy}\sin(k) & -2t_x\cos(k) \end{pmatrix} = 2t_x\cos(k)\sigma_z + [t_y - 2t_{xy}\sin(k)]\sigma_x \tag{3.10}$$

Using transformation matrix $U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}$, we change Hamiltonian to following form:

$$\mathcal{H}_T = U^\dagger \mathcal{H} U = 2t_x\cos(k)\sigma_x + [t_y - 2t_{xy}\sin(k)]\sigma_y \tag{3.11}$$

or

$$\mathcal{H}_T = \begin{pmatrix} 0 & 2t_x\cos(k) - i[t_y - 2t_{xy}\sin(k)] \\ 2t_x\cos(k) + i[t_y - 2t_{xy}\sin(k)] & 0 \end{pmatrix}. \tag{3.12}$$

We take q to be:

$$q = 2t_x\cos(k) - i[t_y - 2t_{xy}\sin(k)], \tag{3.13}$$

winding number and the possible constraints over hopping terms are given in the following,

$$\frac{i}{2\pi}\int_{-\pi}^{+\pi} \frac{1}{q(k)}\frac{\partial q(k)}{\partial k}dk = \frac{i}{2\pi}\int_{-\pi}^{+\pi} \frac{-2t_x\sin(k) + i[2t_{xy}\cos(k)]}{2t_x\cos(k) - i[t_y - 2t_{xy}\sin(k)]}dk \tag{3.14}$$

by setting $t_x = t_{xy} = 1$ we have,

$$\frac{i}{2\pi}\int_{-\pi}^{+\pi} \frac{-2t_x\sin(k) + i[2t_{xy}\cos(k)]}{2t_x\cos(k) - i[t_y - 2t_{xy}\sin(k)]}dk = \frac{i}{2\pi}\int_{-\pi}^{+\pi} \frac{-2\sin(k) + i[2\cos(k)]}{2\cos(k) - i[t_y - 2\sin(k)]}dk$$

$$= \frac{(i)(2i)}{2\pi}\int_{-\pi}^{+\pi} \frac{\exp(ik)}{2\exp(ik) - it_y}dk \tag{3.15}$$

If we change variable in the form $\exp(ik) = z$, then:

$$\frac{2i}{2\times 2\pi}\oint \frac{dz}{z-it_y/2} = \frac{2i}{2\times 2\pi}\times(2\pi i)\lim_{z\to it_y/2}(z-it_y/2)\frac{1}{z-it_y/2} = \frac{2i(2\pi i)}{2\times 2\pi} = -1, \tag{3.16}$$

here, winding number is a negative integer and it implies the existence of a topological invariant. It also exhibits the constraint over t_y: $|t_y/2| < 1 \longrightarrow |t_y| < 2$ in order to have winding number of -1 .

In our ladder structure, using open boundary condition, we can see the degenerate edge states at values greater than $t_{xy} > 0.5$ and smaller than $t_{xy} < -0.5$. To plot the edge states we took the advantage of the Hamiltonian representation in position space(Fig. 3.3),

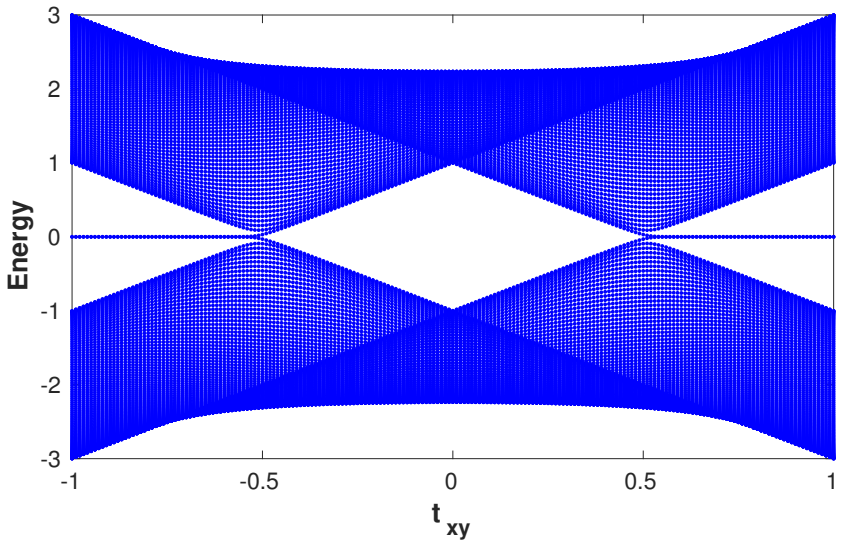


Figure 3.3: Edge states in shifted Creutz model with 200 chains in an open boundary condition.; $t_x = 1$ and $t_y = 1$.

Two degenerate wavefunctions [7] with 0 energies in position space representation of the Hamiltonian is depicted as Fig.3.4. These wavefunctions exhibit the probable position of the hopping electrons.

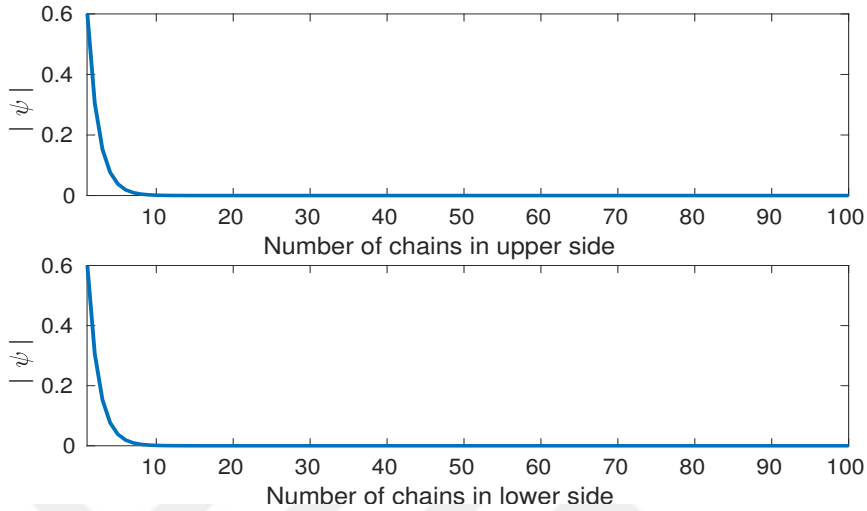


Figure 3.4: End states are plotted for 100 upper and lower chains in an open boundary condition.

According to phase diagram 3.5, a quantum phase transition is occurring while the electron energy crosses the gap closure.

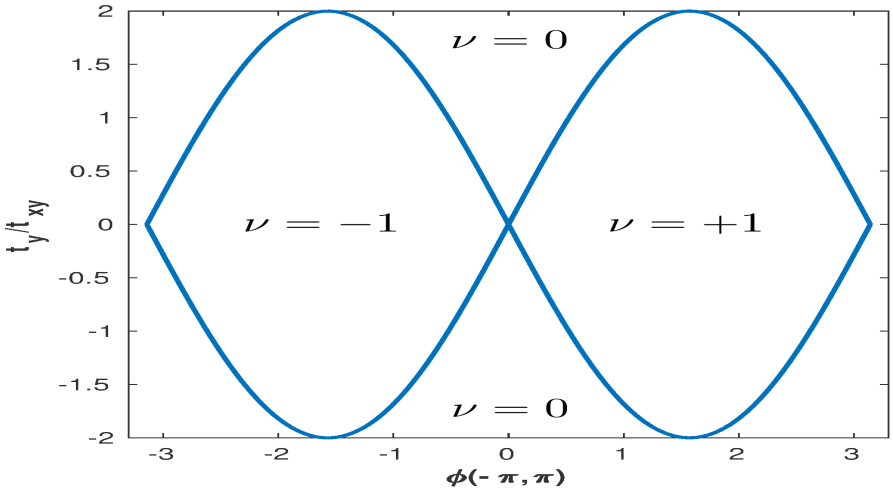


Figure 3.5: Phase diagram of shifted Creutz model with spinless electron model. Hopping terms of vertical and diagonal bonds are varying with the restriction $|t_y/t_{xy}| \leq 2$.

3.2.2 Time reversal, Particle-hole symmetry

Let us consider shifted Creutz model once more,

$$\mathcal{H}(k) = 2t_x \cos(k)\sigma_z + [t_y - 2t_{xy}\sin(k)]\sigma_x \tag{3.17}$$

Time-reversal [8] is represented by an anti-unitary operator,

$$T = U_T K \tag{3.18}$$

where U_T is unitary and K is complex conjugate operator. We assume the unitary part to be $U_T = i\sigma_y$,

$$T = U_T K = i\sigma_y K. \tag{3.19}$$

The $\mathcal{H}(k)$ is transformed as,

$$\begin{aligned}
T\mathcal{H}(k)T^{-1} &= T\{2t_x\cos(k)\sigma_z\}T^{-1} + T\{[t_y - 2t_{xy}\sin(k)]\sigma_x\}T^{-1} \\
&= 2t_x\cos(-k)T\{\sigma_z\}T^{-1} + [t_y - 2t_{xy}\sin(-k)]T\{\sigma_x\}T^{-1} \\
&= 2t_x\cos(k)i\sigma_y K\sigma_z(-i)\sigma_y K + [t_y + 2t_{xy}\sin(k)]i\sigma_y K\sigma_x(-i)\sigma_y K \\
&= 2t_x\cos(k)i\sigma_y\sigma_z(i)\sigma_y^* + [t_y + 2t_{xy}\sin(k)]i\sigma_y\sigma_x(i)\sigma_y^* \\
&= 2t_x\cos(k)\sigma_y\sigma_z\sigma_y + [t_y + 2t_{xy}\sin(k)]\sigma_y\sigma_x\sigma_y \\
&= 2t_x\cos(k)(-\sigma_z) + [t_y + 2t_{xy}\sin(k)](-\sigma_x)
\end{aligned} \tag{3.20}$$

or

$$T\mathcal{H}(k)T^{-1} = \begin{pmatrix} -2t_x\cos(k) & -t_y - 2t_{xy}\sin(k) \\ -t_y - 2t_{xy}\sin(k) & 2t_x\cos(k) \end{pmatrix}. \tag{3.21}$$

Eigenvalues of $\mathcal{H}(k)$ is given by,

$$E(k) = \pm\sqrt{(2t_x\cos(k))^2 + (t_y - 2t_{xy}\sin(k))^2} \tag{3.22}$$

and $T\mathcal{H}(k)T^{-1}$,

$$E(k) = \pm\sqrt{(2t_x\cos(k))^2 + (t_y + 2t_{xy}\sin(k))^2}. \tag{3.23}$$

Obtained eigenvalues for $\mathcal{H}(k)$ and $T\mathcal{H}(k)T^{-1}$ are having different values. Hence the Hamiltonian is not invariant under time reversal transformation. Particle-hole symmetry $C = U_C K$ is similar to time-reversal, it has a unitary part and a complex conjugate part where if it holds, then it needs to satisfy:

$$U_C\mathcal{H}^*_{-k}{U_C}^{-1} = -\mathcal{H}_k, \tag{3.24}$$

the symmetry analysis for particle-hole operator would follow similar steps as time reversal and it would not satisfy equation 3.24.

3.2.3 Chiral symmetry

Chiral anti-symmetry operator $S = TC$ is another symmetry that our Hamiltonian can possess it. If it holds, it is necessary to confirm this:

$$U_S \mathcal{H}_k U_S^{-1} = -\mathcal{H}_k \tag{3.25}$$

If we choose $U_S = \sigma_y$, then we have,

$$\sigma_y \sigma_z \sigma_y^{-1} \to -\sigma_z \qquad\qquad \sigma_y \sigma_x \sigma_y^{-1} \to -\sigma_x \tag{3.26}$$

considering equation 3.17, it confirms the required condition. Since $TT = 0$, $CC = 0$ and $SS = 1$, from periodic table of topological structures [9, 10], it can be confirmed that our toy model holds the topological index of $\mathbb{Z}$ with label of AIII.

3.3 Shifted Creutz model with spin-orbit and Rashba coupling terms

Using the introduced Hamiltonian by Kane-Mele [5], we can include spin-orbit interaction in our model. The Hamiltonian is,

$$H = -t \sum_{\langle i,j\rangle\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} \quad - \quad i t_{xy} \sum_{\langle\langle i,j\rangle\rangle\alpha\beta} c_{i\alpha}^{\dagger} v_{ij} \sigma_{\alpha\beta}^{z} c_{j\beta} \quad - \quad i\lambda_R \sum_{\langle i,j\rangle\alpha\beta} c_{i\alpha}^{\dagger} \left(\boldsymbol{\sigma}_{\alpha\beta} \times \mathbf{d}_{ij}\right)_z c_{j\beta}. \tag{3.27}$$

In the first term, hopping term is for horizontal and vertical bonds, while hopping term for second term is for diagonal bonds. In the second term, v_{ij} represents the induced phase on the diagonal bonds. As usual, $\langle i,j\rangle$ indicates that i and j are nearest-neighbor sites while $\langle\langle i,j\rangle\rangle$ refers to second-nearest neighbors. The

vector $\mathbf{d_{ij}}$ represents the corresponding vector pointing from i to j and it is only for nearest-neighbor sites. The third term of Hamiltonian is Rashba SO interaction term where it is for nearest-neighbor sites and it has explicit spin dependence.

$$H = H_1 + H_2 + H_3 \tag{3.28}$$

where each H_i corresponds respectively to one of the three terms of Hamiltonian. Now, let's rewrite shifted Creutz model in position space while spin-orbit coupling is included,

$$\begin{aligned} H_1 = -\sum_n [& t_x(a^\dagger_{n\uparrow}a_{n+1\uparrow} + a^\dagger_{n+1\uparrow}a_{n\uparrow} + a^\dagger_{n\downarrow}a_{n+1\downarrow} + a^\dagger_{n+1\downarrow}a_{n\downarrow}) \\ & - t_x(b^\dagger_{n\uparrow}b_{n+1\uparrow} + b^\dagger_{n+1\uparrow}b_{n\uparrow} + b^\dagger_{n\downarrow}b_{n+1\downarrow} + b^\dagger_{n+1\downarrow}b_{n\downarrow}) \\ & + t_y(a^\dagger_{n\uparrow}b_{n\uparrow} + b^\dagger_{n\uparrow}a_{n\uparrow} + a^\dagger_{n\downarrow}b_{n\downarrow} + b^\dagger_{n\downarrow}a_{n\downarrow})], \end{aligned} \tag{3.29}$$

the second term is,

$$\begin{aligned} H_2 = & -it_{xy}\sum_n(-a^\dagger_{n\uparrow}b_{n+1\uparrow} + a^\dagger_{n\downarrow}b_{n+1\downarrow} + a^\dagger_{n+1\uparrow}b_{n\uparrow} - a^\dagger_{n+1\downarrow}b_{n\downarrow} \\ & + b^\dagger_{n+1\uparrow}a_{n\uparrow} - b^\dagger_{n+1\downarrow}a_{n\downarrow} - b^\dagger_{n\uparrow}a_{n+1\uparrow} + b^\dagger_{n\downarrow}a_{n+1\downarrow}) \end{aligned} \tag{3.30}$$

and finally we have,

$$\begin{aligned} H_3 = & -i\lambda_R\Big[ia^\dagger_{n\uparrow}a_{n+1\downarrow} - ia^\dagger_{n\downarrow}a_{n+1\uparrow} + ia^\dagger_{n+1\downarrow}a_{n\uparrow} - ia^\dagger_{n+1\uparrow}a_{n\downarrow} \\ & + ib^\dagger_{n\uparrow}b_{n+1\downarrow} - b^\dagger_{n\downarrow}ib_{n+1\uparrow} + ib^\dagger_{n+1\downarrow}b_{n\uparrow} - ib^\dagger_{n+1\uparrow}b_{n\downarrow} \\ & - a^\dagger_{n\uparrow}b_{n\downarrow} - a^\dagger_{n\downarrow}b_{n\uparrow} + b^\dagger_{n\uparrow}a_{n\downarrow} + b^\dagger_{n\downarrow}a_{n\uparrow}\Big] \end{aligned} \tag{3.31}$$

Using Fourier transform at 3.4, we can represent our Hamiltonian in k space. The matrix representation of Hamiltonian is given by:

$$H(k) = -(a^{\dagger}_{k\uparrow} \quad a^{\dagger}_{k\downarrow} \quad b^{\dagger}_{k\uparrow} \quad b^{\dagger}_{k\downarrow}) \quad \mathcal{H}(k) \quad \begin{pmatrix} a_{k\uparrow} \\ a_{k\downarrow} \\ b_{k\uparrow} \\ b_{k\downarrow} \end{pmatrix} \tag{3.32}$$

where $\mathcal{H}(k)$ is the kernel of Hamiltonian.

$$\mathcal{H}(k) = \begin{pmatrix} 2t_x\cos(k) & 2i\lambda_R\sin(k) & t_y - 2t_{xy}\sin(k) & -i\lambda_R \\ -2i\lambda_R\sin(k) & 2t_x\cos(k) & -i\lambda_R & t_y + 2t_{xy}\sin(k) \\ t_y - 2t_{xy}\sin(k) & i\lambda_R & -2t_x\cos(k) & 2i\lambda_R\sin(k) \\ i\lambda_R & t_y + 2t_{xy}\sin(k) & -2i\lambda_R\sin(k) & -2t_x\cos(k) \end{pmatrix} \tag{3.33}$$

If we plot the band structure for recent matrix, there can be seen two states with time-reversal invariant momenta at points k and $-k$ where they are two-fold degenerate which is consistent with Kramer's theorem.

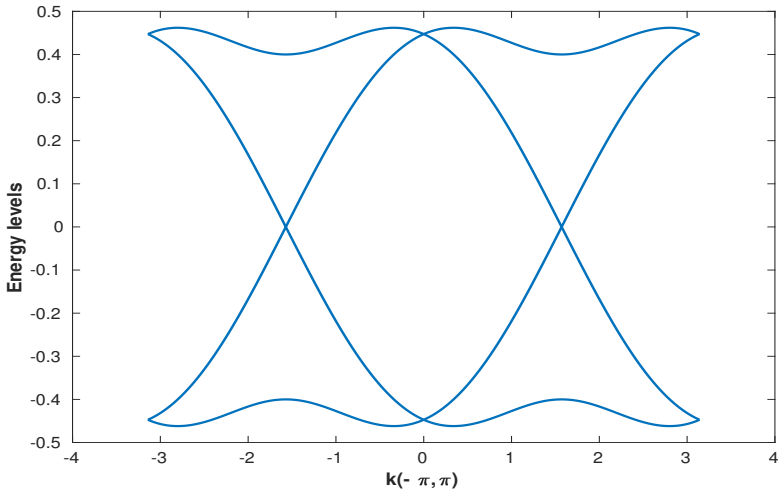


Figure 3.6: Energy band structure; Rashba term is off. The values are set as $t_x = 0.2$, $t_{xy} = 0.1$, and $t_y = 0.2$ in a periodic boundary condition.

When we turn on Rashba term, a gap appears in the band structure, but we

can close this gap by resetting the hopping terms.

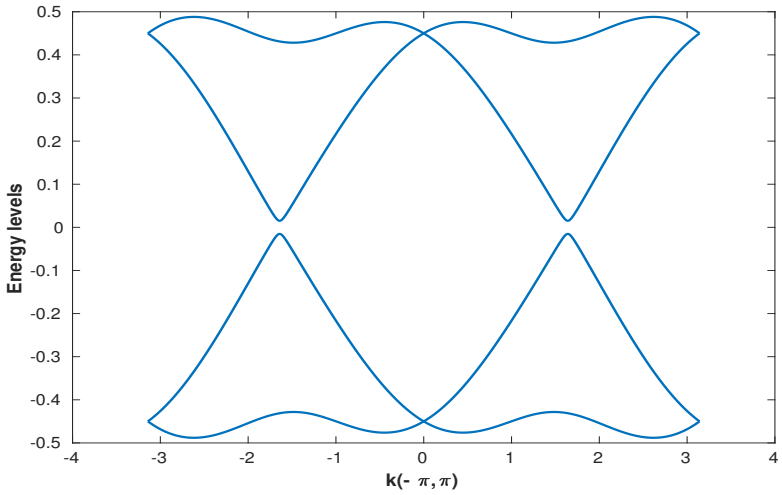


Figure 3.7: Energy band structure; Rashba term is on. The values are set as $t_x = 0.2$, $t_{xy} = 0.1$, $t_y = 0.2$, and $\lambda_R = 0.1$ in a periodic boundary condition.

While spin-orbit interaction is considered, still there exists edge states. To plot edge states, we used the open boundary condition.

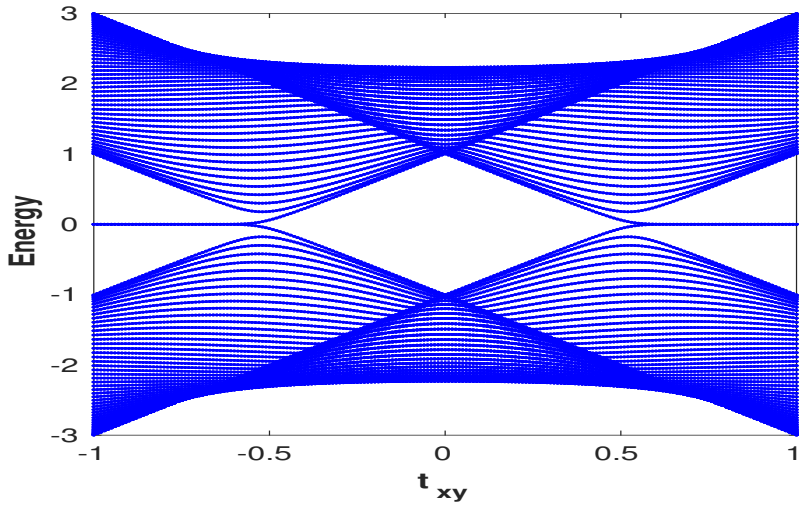


Figure 3.8: Edge states while spin-orbit interaction is included; Rashba term is off. The values set as $t_x = 1$, $t_y = 1$ for 200 chains.

3.3.1 Time reversal symmetry

When spin-orbit and Rashba SO coupling is being taken into account, the kernel of Hamiltonian is given by,

$$\mathcal{H}(k) = \begin{pmatrix} 2t_x\cos(k) & 2i\lambda_R\sin(k) & t_y - 2t_{xy}\sin(k) & -i\lambda_R \\ -2i\lambda_R\sin(k) & 2t_x\cos(k) & -i\lambda_R & t_y + 2t_{xy}\sin(k) \\ t_y - 2t_{xy}\sin(k) & i\lambda_R & -2t_x\cos(k) & 2i\lambda_R\sin(k) \\ i\lambda_R & t_y + 2t_{xy}\sin(k) & -2i\lambda_R\sin(k) & -2t_x\cos(k) \end{pmatrix}. \tag{3.34}$$

$\mathcal{H}(k)$ can be expressed in terms of Dirac matrices,

$$\mathcal{H}(k) = -\sum_{a=1}^{5} d_a(k)\Gamma^a - \sum_{a<b=1}^{5} d_{ab}(k)\Gamma^{ab} \tag{3.35}$$

where the five Dirac matrices are given by:

$$\Gamma^a = (\sigma_x \otimes s_0, \sigma_z \otimes s_0, \sigma_y \otimes s_x, \sigma_y \otimes s_y, \sigma_y \otimes s_z) \tag{3.36}$$

and $a = 1, 2, 3, 4, 5$. The commutators of Dirac matrices can be obtained by following commutation relation:

$$\Gamma^{ab} = \frac{1}{2i}[\Gamma^a, \Gamma^b]. \tag{3.37}$$

Time reversal operator could be taken as $T = i(\sigma_0 \otimes s_y)K$ in the existing representation. Dirac matrices and its commutators are even and odd respectively under time reversal transformation:

$$\begin{aligned} T\Gamma^a T^{-1} &= \Gamma^a, \\ T\Gamma^{ab} T^{-1} &= -\Gamma^{ab} \end{aligned} \tag{3.38}$$

It is easy to see that the given Hamiltonian is time reversal invariant, since the Dirac matrices coefficients are respectively even and odd as well:

$$\begin{aligned} d_a(-k) &= d_a(k), \\ d_{ab}(-k) &= -d_{ab}(k) \end{aligned} \tag{3.39}$$

where

$$d_1 = t_y \qquad d_2 = 2t_x\cos(k) \qquad d_3 = \lambda_R$$
$$d_{25} = 2t_{xy}\sin(k) \qquad d_{35} = 2\lambda_R\sin(k).$$

3.3.2 Particle-hole symmetry

Particle-hole is anti-unitary operator. Hence it can be written as combination of a unitary part and a complex conjugate part.

$$C\mathcal{H}C^{-1} = (U_C K)\mathcal{H}_k(U_C K)^{-1} = U_C K\mathcal{H}_k K^{-1}{U_C}^{-1} = U_C\mathcal{H}^*_{-k}{U_C}^{-1} \tag{3.40}$$

Therefore it is enough to show:

$$U_C\mathcal{H}^*_{-k}{U_C}^{-1} = -\mathcal{H}_k \tag{3.41}$$

If we consider $C = (\sigma_y \otimes \sigma_x)K$, then $U_C = \sigma_y \otimes \sigma_x$ and,

$$U_C[d_1(-k)\gamma^{1*}]U_C^{-1} = -d_1(k)\gamma^1 \qquad U_C[d_2(-k)\gamma^{2*}]U_C^{-1} = -d_2(k)\gamma^2$$
$$U_C[d_3(-k)\gamma^{3*}]U_C^{-1} = -d_3(k)\gamma^3 \qquad U_C[d_{25}(-k)\gamma^{25*}]U_C^{-1} = -d_{25}(k)\gamma^{25}$$
$$U_C[d_{35}(-k)\gamma^{35*}]U_C^{-1} = -d_{35}(k)\gamma^{35}$$

which confirms equation 3.41. And particle-hole anti-unitary operator satisfies:

$$CC = U_C K U_C K = (\sigma_y \otimes \sigma_x)K(\sigma_y \otimes \sigma_x)K = (\sigma_y \otimes \sigma_x)(\sigma_y^* \otimes \sigma_x) = -1 \tag{3.42}$$

3.3.3 Chiral symmetry

Chiral anti-symmetry operator is defined as $S = TC$, hence we can write,

$$S = TC = U_T K U_C K = U_T U_C^* = U_S, \tag{3.43}$$

thus for transformation we have,

$$\begin{aligned} S\mathcal{H}_k S^{-1} &= U_S\mathcal{H}_k U_S^{-1} = (U_T U_C^*)\mathcal{H}_k(U_T U_C^*)^{-1} \\ &= [i(\sigma_0 \otimes s_y)(\sigma_y^* \otimes \sigma_x)]\mathcal{H}_k[i(\sigma_0 \otimes s_y)(\sigma_y^* \otimes \sigma_x)]^{-1} \\ &= [i(\sigma_0 \otimes s_y)(-\sigma_y \otimes \sigma_x)]\mathcal{H}_k[i(\sigma_0 \otimes s_y)(-\sigma_y \otimes \sigma_x)]^{-1} \\ &= [i(\sigma_0 \otimes s_y)(-\sigma_y \otimes \sigma_x)]\mathcal{H}_k\big\{(-\sigma_y \otimes \sigma_x)[-i(\sigma_0 \otimes s_y)]\big\} \end{aligned} \tag{3.44}$$

So, it is enough to show that,

$$S\mathcal{H}_k S^{-1} = -\mathcal{H}_k, \tag{3.45}$$

if we replace $\mathcal{H}_k$ with its components, then,

$$\begin{aligned} U_S[d_1(k)\gamma^1]U_S^{-1} &= -d_1(k)\gamma^1 & U_S[d_2(k)\gamma^2]U_S^{-1} &= -d_2(k)\gamma^2 \\ U_S[d_3(k)\gamma^3]U_S^{-1} &= -d_3(k)\gamma^3 & U_S[d_{25}(k)\gamma^{25}]U_S^{-1} &= -d_{25}(k)\gamma^{25} \\ U_S[d_{35}(k)\gamma^{35}]U_S^{-1} &= -d_{35}(k)\gamma^{35} \end{aligned}$$

where confirms existence of chiral symmetry. Now, let's find SS value,

$$SS = U_T U_C^* U_T U_C^* = i(\sigma_0 \otimes s_y)(\sigma_y^* \otimes \sigma_x) i(\sigma_0 \otimes s_y)(\sigma_y^* \otimes \sigma_x) = 1 \tag{3.46}$$

Since we have $TT = -1$, $CC = -1$ and $SS = 1$, according to periodic table of topological structures [9], our Hamiltonian holds $2\mathbb{Z}$ topological index with CII label.

Chapter 4

Conclusion

We studied Bloch-type functions for a lattice in presence of a uniform magnetic field resulted from commutation of modified translation operaotrs with the Hamiltonian of the system, firstly introduced by E. Brown [1] and then extended by J.Zak [2]. We learned how to form full groups rather than ray groups by manipulating the translation operators. We utilized the same idea, and showed that the same idea can be applied to a set of translation operators in phase space coordinate which contains both translation in position and momentum spaces. These translation operators form a ray group but they can be modified to form a full group by adding an extra term consisting of different paths which gives the same displacement vector. During chapter 3, we studied the Creutz model and learned about the cross-linked ladder and its band structures. By using this model, we introduced a toy model and calculated the band structures and its possible symmetries. Then by utilizing the Kane-Mele [5, 4] idea, we rewrite the Hamiltonian for our toy model while spin orbit interaction is included. Expressing our Hamiltonian in terms of Dirac matrices, we were able to show the possible symmetries in the system. These symmetries help us to interpret the different aspects of the system, most importantly the energy structure. We demonstrate the topological behavior via an investigation of the band structure, characteristic edge states, and investigate the transport properties.

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Appendix A

Mathematical Background

A.1 Basics of group and representation theory

Definition. A group G [11, 12] is defined as a set closed under a binary operation $*$ such that following axioms to be satisfied:

1. For all elements $a, b, c \in G$ there is,
   $(a * b) * c = a * (b * c)$ (Associativity)
2. There is an element denoted with $e \in G$ where for all elements $a \in G$ we have,
   $e * a = a * e$ (Identity element)
3. For each $a \in G$, in correspondent there exist another element like $a' \in G$ such that,
   $a * a' = a' * a = e$ (Inverse element)

Definition. A subgroup H is a subset of group G where it is closed under the binary operation $*$ of G and it forms a group by same operation.

Theorem. A subgroup H of G should satisfy following axioms:

1. H is closed under binary operation of G

2. The identity element of G is in H

3. For every element of H there exists its inverse element too.

Definition. A map ϕ from group $(G, *)$ to $(G', \cdot)$ is a homomorphism if it satisfies,

$$\phi(a * b) = \phi(a) \cdot \phi(b) \tag{A.1}$$

for all $a, b \in G$.

Definition. A map ϕ from group $(G, *)$ to $(G', \cdot)$ is an isomorphism if it is bijective between two groups and also satisfies,

$$\phi(a * b) = \phi(a) \cdot \phi(b) \tag{A.2}$$

for all $a, b \in G$.

Group representation. Let's assume there are operators $A, B, ...$ in a vector space L. If the operators form a group, according to the above definitions, then we can map elements of group G on operators in vector space L. Identity element of G will be mapped on identity operator in vector space L, and all operators in L have the inverse operator. The map from arbitrary group G to vector space L is generally homomorphic and if R and S belongs to group G then the corresponding operators in vector space L will be $D(R)$ and $D(S)$ where are satisfying:

$$\begin{aligned} &D(RS) = D(R)D(S) \\ &D(R^{-1}) = D(R)^{-1} \\ &D(E) = 1. \end{aligned} \tag{A.3}$$

$D(G)$ is called the representation of group G in the representation space L. If we restrict our vector space L to linear spaces, then by choosing a proper basis we can construct a matrix representation for each $D(G)$.

Equivalent representations. If we change the basis that our matrix representation $D(R)$ is constructed based on, then, the obtained matrix can be

expressed in terms of former matrix transformation,

$$D'(R) = CD(R)C^{-1} \tag{A.4}$$

where provides another representation for group G. Since $D'(R)$ has the same trace as $D(R)$, it is called an equivalent representation of $D(R)$.